# THE POLARON HYDROGENIC ATOM IN A STRONG MAGNETIC FIELD

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Rohan Ghanta

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# THE POLARON HYDROGENIC ATOM IN A STRONG MAGNETIC FIELD

Approved by:

Dr. Michael Loss, Advisor
School of Mathematics
*Georgia Institute of Technology*

Dr. Federico Bonetto
School of Mathematics
*Georgia Institute of Technology*

Dr. Rafael de la Llave
School of Mathematics
*Georgia Institute of Technology*

Dr. Evans Harrell
School of Mathematics
*Georgia Institute of Technology*

Dr. Brian Kennedy
School of Physics
*Georgia Institute of Technology*

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"An electron moving moving with its accompanying distortion of the lattice has sometimes been called a polaron. It has an effective mass higher than that of the electron. We wish to compute the energy and effective mass of such an electron. A summary giving the present state of this problem has been given by Fröhlich. He makes simplifying assumptions, such that the crystal lattice acts like a dielectric medium, and that all the important phonon waves have the same frequency. We will not discuss the validity of these assumptions here, but will consider the problem described by Fröhlich as simply a mathematical problem."

R.P. Feynman, "Slow Electrons in a Polar Crystal," (1954).

"However, Feynman's method is rather complicated, requiring the services of the Massachusetts Institute of Technology Whirlwind computer, and moreover suffers from a lack of directness. It is not clear how to relate his method to more pedestrian manipulations of Hamiltonians and wave functions."

E.H. Lieb and K. Yamazaki, "Ground-State Energy and Effective Mass of the Polaron," (1958).

To my family.

Acknowledgement

I consider it my pleasant duty to express my deepest gratitude to Michael Loss for his guidance over the years and for providing me with an opportunity to pursue my interests and work on the polaron, which has been a great source of joy in my life.

I would like to thank Federico Bonetto, Rafael de la Llave, Evans Harrell and Brian Kennedy for serving on the thesis committee. I am grateful to the National Science Foundation for support.

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## Summary

It is shown that: (1) The ground-state electron density of a polaron bound in a Coulomb potential and exposed to a homogeneous magnetic field of strength $B$–with its transverse electron coordinates integrated out and when scaled appropriately with the magnetic field strength–converges pointwise and in a weak sense as $B \to \infty$ to the square of a hyperbolic secant function; (2) The ground state of a polaron bound in a symmetric Mexican hat-type potential, scaled appropriately with the electron-phonon coupling parameter, is unique and therefore rotation-invariant, but the minimizers of the corresponding Pekar problem are nonradial; in the strong-coupling limit under the assumption that these minimizers are unique up to rotation the ground-state electron density–when scaled appropriately with the electron-phonon coupling strength–converges in a weak sense to a rotational average of their densities.

CHAPTER 1

# Introduction

## 1.1. The Development of the Polaron Concept

An electron moving in an ionic crystal polarizes the surrounding lattice by exciting its phonon modes[1]–the collective vibrational displacements of the ions from their equilibrium positions–and carries with it a polarization cloud of phonons. An electron dressed with its polarization cloud is known as a *polaron*.[2] It is heavier and less mobile than the bare electron and has been fundamental to understanding the physics of semiconductors. Being one of the simplest examples of a particle interacting with a quantized field the polaron has served as a testing ground for various techniques in Quantum Field Theory during the 1950s–a notable example is R.P. Feynman's now-ubiquitous path integral [**Fy1955**]–undoubtedly the Golden Age of polaron theory. Moreover in recent years the polaron concept has experienced a renewed interest due to experimental advances in ultracold quantum gases, which will fuel further developments in polaron theory in the years to come.[3]

[1]The term *phonon* is derived from the Greek word for sound since phonons can give rise to sound waves in an ionic crystal. The concept was introduced by the Soviet physicist I. Tamm in 1932 [**Tm1932**] for which he is featured on the Russian postage stamp from 2000 with the inscription (in Russian) "Idea of Phonons, 1929." An analogous concept in Quantum Electrodynamics is a *photon* describing a quanta of light. Tamm's student S.I. Pekar was one of the pioneers of polaron theory.

[2]The term *polaron* was coined by S.I. Pekar in 1946 [**Pk1946**].

[3]In 2016 researchers at Aarhus University have demonstrated the existence of a *Bose polaron*, describing a mobile impurity in a Bose-Einstein condensate [**Jg2016**]. In 2017 M. Lemeschko at the Institute of Science

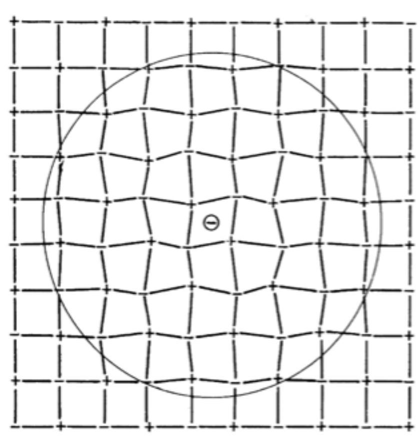

FIGURE 1.1.1. A polaron is a quasiparticle consisting of an electron together with its polarization cloud of virtual phonons in an ionic crystal. Extensions of the polaron concept have appeared in recent years to describe an impurity in Bose-Einstein condensates of ultracold atoms, for example, the *Bose polaron* [**Jg2016**], the *angulon* [**Lm2017**] and the *Rydberg polaron* [**Cm2018**].

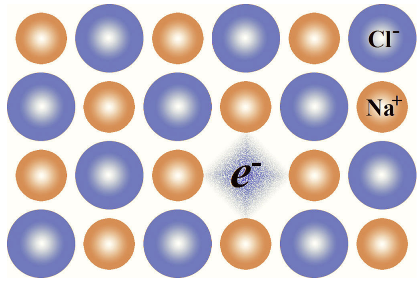


FIGURE 1.1.2. The above figure illustrates a F-center in NaCl. A F-center is a crystallographic defect where an ionic vacancy in the lattice is filled by an electron. In 1933 L.D. Landau suggested that a F-center emerges from an electron trapping itself in its own polarization cloud [**Ld1933**]. The existence of self-trapping in various polaron models is still under active debate.

The roots of polaron theory begin in 1933 in L.D. Landau's one-page paper where it has been suggested that lattice defects such as a F-center in NaCl can arise from an electron being trapped in a phonon hole of its own making [**Ld1933**]. It cannot be emphasized enough the long-lasting influence Landau's rather short and speculative paper has had on polaron physics. There Landau has fired the first shot in what has become a full-fledged and still-active debate on whether polarons indeed exhibit self-trapping. This is one of the most important problems in polaron theory going back to the very origin of the polaron concept itself and not surprisingly has attracted several generations of physicists. Furthermore it was Landau's note that inspired S.I. Pekar in the 1940s to develop a nonlinear theory of the polaron as a self-trapped state [**Pk1951**].[4] The previous two remarks shall be addressed deservingly in more detail below. Meanwhile in Bristol the German physicist H. Fröhlich,[5]

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and Technology in Austria has demonstrated the existence of the *angulon* in Superfluid Helium [**Lm2017**]. Known as the "rotational polaron," the angulon is a quasiparticle consisting of a quantum rotor dressed with a many-particle field of Bosonic excitations. In 2018 researchers at Rice University's Center for Quantum Materials in Houston experimentally realized the *Rydberg polaron* by exciting a Rydberg atom in a Strontium Bose-Einstein condensate [**Cm2018**]. The radius of the excited Rydberg atom is so large that in between its nucleus and the excited electron's orbit lay several Strontium atoms. The electron scatters at the Strontium atoms thereby creating a weak bond between the excited Rydberg atom and the Strontium atoms. The Rydberg atom dressed with the Strontium atoms is known as the Rydberg polaron.

[4] In the Introduction to his 1951 manuscript [**Pk1951**] S.I. Pekar writes "...in 1933 L.D. Landau advanced the important idea of autolocalization of the electron in an ideal crystal as a result of the deformation of the lattice by the field of the electron itself. These local states were assumed to be immobile, and Landau attemmpted to identify them with F-centers in colored alkali-halide crystals. In 1936, Y.a. I. Frenkel' noted that the conduction electron should deform the crystal atoms closest to it and that this local deformation should move in the crystal and follow the electron. In 1936, D.I. Blokhintsev made an attempt to explain on the basis of the approximation of strongly bound electrons in which crystals one should expect the autolocalization of the electrons, indicated earlier by Landau, to be realized. At that time it was impossible to find a correct way for considering autolocal states, and therefore it was impossible to prove their existence and to investigate their properties. These articles, however, had a certain influence on the author's work in this field."

[5] In 1932 Herbert Fröhlich (1905-1991) became a Privatdozent at Albert-Ludwigs-Universität Freiburg, but was dismissed from his position in 1933 due to Hitler's *Berufsbeamtengesetz.* In 1934 he accepted a position at the Ioffe Institute in Leningrad, but in 1935 he fled Russia to England during the Great Purge. (On the other hand L.D. Landau, also one of the pioneers of polaron theory, was unfortunately imprisoned during the Great Purge [**Gr1997**].) In 1937 Neville Francis Mott offered Fröhlich a position at Bristol, where he

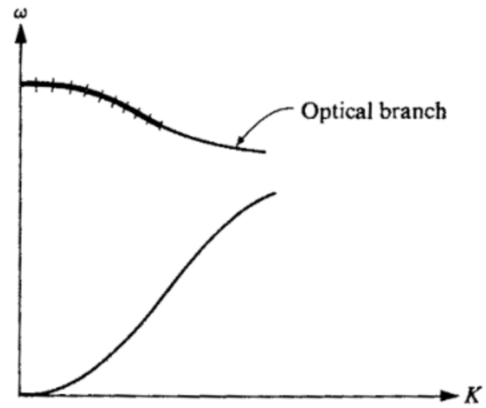


FIGURE 1.1.3. The above plot describes the relationship between phonon wave number $K$ and frequency $\omega$. There are two branches: a branch of optical phonons with a higher and "nearly equal" frequency and a branch of acoustic phonons with lower frequency. In his model Fröhlich only considers the interaction with the optical modes, which are assumed to all have the same frequency.

dissatisfied with the existing theories of dielectric breakdown in ionic crystals and motivated by von Hippel's experiments in the 1930s, developed a theory in 1937 explaining breakdown as mediated by the interaction between the electron and the quantized phonon modes of the crystal [**Fr1937**].[6] There Fröhlich has proposed a polaron model which now bears his name. He has made several simplifying assumptions for example that the electron only excites the optical phonon modes, i.e. the two neighboring ions of opposite sign vibrate in opposite directions, and that these modes all have the same frequency.[7] Furthermore it follows from his derivation of the polaron Hamiltonian that the electron interacts only with the *longitudinal*

published his first book on dielectrics [**Fr1936**]. Aside from his internment in 1940 at Somerset as a *Class C* "enemy" alien, Fröhlich remained in Bristol pursuing a research program on the dielectric breakdown in solids until 1948, when he accepted a position as the Chair of Theoretical Physics at Liverpool. At Liverpool Fröhlich established a research group with several members and visitors including G.R. Allcock, A.B. Bhatia, M. Gurari, H. Haken, K. Huang, S. Nakajima, H. Pelzer and S. Zienau, who have all made important contributions to polaron theory. See [**Hy2015**].

[6]Dielectric breakdown is the phenomenon where an insulator to which a sufficiently strong electrical field is applied becomes instead a conductor. Prior to the publication of Fröblich's paper [**Fr1937**], the existing theories did not account for the electron-phonon interaction. A mechanical theory had been developed on the assumption that the breakdown is due to imperfections in the crystal but later discredited with experiments performed by von Hippel [**vH1932**]. Another theory had been developed by Joffé et.al who proposed that the breakdown is due to the ionization of the ions by the moving ions [**JKS1927**]. This too was discredited as experiments performed in 1935 by von Hippel showed that such a theory was not consistent with the short time scale on which the breakdown takes place [**vH1935**]. It was von Hippel's suggestion that the breakdown is due to the polarization of the lattice by the electrons in the conduction band which inspired Fröhlich to propose the first polaron model.

[7]The vibrational modes of an ionic crystal can be classified as either optical phonons or acoustic phonons [**Ta1961**], [**ST1973**] which describe two neighboring ions of opposite sign vibrating in the same direction. The optical modes therefore correspond to polarization waves with a much larger wavelength. For this reason alone Fröhlich found it appropriate to consider only the interaction with optical phonons. Furthermore, in an ionic crystal the optical modes all have nearly the same frequency. See Figure 1.1.3.

optical modes and that the interaction is Coulombic. The Fröhlich Hamiltonian is a sum of three operators: that of the kinetic energy of the electron, that of the energy of the phonon modes–treated as harmonic oscillators–and that of the electron-phonon interaction energy. As shall be discussed in more detail below, Fröhlich has returned to the model but with a completely different motivation during the 1950s when the flourishing field of Quantum Electrodynamics was facing some serious mathematical difficulties.

About a decade later in 1946 at the Academy of Sciences of the Ukranian SSR in Kiev the physicist S.I. Pekar[8] having realized the inadequacy[9] of the standard band theory of that time derived independently of Fröhlich the same polaron model. Whereas Fröhlich's main concern was calculating the breakdown field in dielectric materials, Pekar set out to determine the energy spectrum of the polaron. It was immediately clear that the electron-phonon interaction term in the Hamiltonian makes calculating even the ground-state energy intractable. To work around this mathematical difficulty Pekar found inspiration in Landau's short note [**Ld1933**] suggesting that an electron traps itself in its own phonon cloud. Indeed it was Pekar who using the adiabatic formalism first described how such self-trapping can occur: the phonons not being able to follow the rapidly moving electron form a potential well deep enough to localize it.[10] Based on this feeling that the phonons cannot be sensitive to the instantaneous position of the relatively fast electron–but instead interact with its "mean" electron density–he has made an Ansatz for the ground-state wave function: it has the product form $\psi(\mathbf{x})\Phi$ with $\psi(\mathbf{x})^2$ the probability density of the localized electron and $\Phi$ a phonon coherent state.[11] Pekar's Produkt-Ansatz provides the computational convenience of eliminating all of the phonon coordinates in the variational calculation for the

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[8]Solomon Isaakovich Pekar (1917-1985) spent his entire career in Kiev, where he was a full member of the Ukranian Academy of Sciences. Around 1946 when he has devised an explanation for the self-trapping of the electron suggested by Landau in [**Ld1933**], his advisor I. Tamm took him to Moscow to present his results at Landau's seminar. According to folklore it was then during the discussion with Landau that the quasiparticle consisting of an electron trapped in its polarization cloud was baptized as "polaron". See [**Kj1999**]. Pekar has made several contributions to condensed matter theory, in particular to the study of crystals, and his research was certainly not restricted to the polaron. For example by the late 1950s he started to work on excitions. In 1960 he co-founded the Institute of Semiconductor Physics of the Ukranian Academy of Sciences in Kiev. See [**Af1986**].

[9]As discussed in [**Pk1951**] the standard band theory of that time described the conduction electron in a semiconductor using the so-called zeroth approximation, which ignores the electron-phonon interaction; when calculating certain quantities such as the diffusion coefficient and electron mobility the electron-phonon interaction is accounted for as a small perturbation. The calculated values such as the energy of thermal dissociations, recombination coefficients, quantum yield of the internal photoeffect were not in agreement with experiment.

[10]Like Landau in [**Ld1933**] Pekar initially considered the polaron to be immobile [**Pk1946**]. But later in [**Pk1947**] and [**Pk1948**] he has advanced the idea of the polaron–and not the band electron–as a charge carrier in an ionic crystal, a significant improvement in semiconductor physics. Together with Landau in [**LP1948**] he proposed a system of non-linear partial differential equations to describe the motion of the polaron as a (localized) charge carrier while accounting for the effective mass of the polaron rather than the bare mass of the band electron. The validity of these evolution equations for describing the true dynamics of the polaron has been examined only recently [**FS2014**], [**FG2017**], [**FG2019**], [**LRSS2019**].

[11]This is also known as the adiabatic or Born-Oppenheimer approximation. When calculating with the Produkt-Ansatz it follows naturally from a completion of the square that the phonon displacements in the coherent state depend on the "mean" electron density $\psi(\mathbf{x})^2$ thereby coupling the electron to the phonon field albeit in a "mean-field" manner. A similar approach is also taken by Evrard, Kartheuser and Devreese [**EKD1970**] when they initiated the study of polarons in strong magnetic fields.

ground-state energy with Pekar arriving at a much simpler albeit nonlinear minimization problem in which the electron-phonon interaction is now replaced by an effective Coulomb self-interaction of the electron; the electronic wave function in his Ansatz is the minimizer of the nonlinear problem. Subsequently in a series of collaborations with M.F. Deigen, Landau[12], Y.E. Perlin and O.F. Tomasevich, Pekar has developed an effective nonlinear theory of the polaron built entirely on his (unjustified!) Ansatz [**DP1948**], [**DP1951**], [**LP1948**], [**PP1950**], [**PT1951**]. These results obtained between 1944 and 1950 in the Ukranian SSR have been conveniently synthesized in Pekar's lucid monograph [**Pk1951**]. Moreover, not being amenable to the direct method in the calculus of variations his effective model has in turn challenged mathematicians to develop novel and far-reaching techniques in nonlinear analysis.[13]

At around the same time that Landau and Pekar's seminal paper [**LP1948**] was published Quantum Electrodynamics was becoming one of the most active areas of research in theoretical physics with the introduction of several renormalization procedures for taming the divergences that have plagued the theory. Being not mathematically sound these renormalization procedures have been criticized heavily by the same people such as P.A.M. Dirac and Feynman[14] who have played a pivotal role in the development of Quantum Electrodynamics. It was during this time that Fröhlich then at Liverpool has turned to his earlier polaron model as the ideal setting for a singularity-free field theory.[15] In 1950 together with H. Pelzer and S. Zienau Fröhlich has considered his 1937 polaron model but with two modifications. In [**FPZ1950**] they have treated the crystal as a dielectric *continuum*, the validity

[12]At the time of his joint work with Pekar on the effective mass of the polaron [**LP1948**] Lev Davidovich Landau (1909-1968) was the head of the Theoretical Division at the Institute for Physical Problems in Moscow. In fact Landau began his career in the Ukranian SSR, where he was the head of the Department of Theoretical Physics at the National Scientific Center Kharkiv Institute of Physics and Technology, about 250 miles from from Kiev. During the Great Purge, Landau was arrested in Khrakiv for circulating a leaflet criticizing Stalin. He promptly left Khrakiv in 1937 for his new position in Moscow but was again arrested and imprisoned from 1938-1939 at the Lubyanka prison in Moscow on same charges. See [**Gr1997**].

[13]The first detailed analysis of Pekar's nonlinear minimization problem was given in 1977 by E.H. Lieb [**Lb1977**] where it is shown using symmetrization arguments that a minimizer exists; uniqueness (up to translations) is also argued. The issue here is that Pekar's problem involves minimizing a nonconvex functional on an unbounded domain: the minimizing sequences can "walk off" to infinity, and this is where symmetric decreasing rearrangements come in handy! (Recall, the electronic wavefunction in Pekar's Produkt Ansatz is a minimizer of the nonlinear problem; Pekar just assumed a minimizer exists.) In order to argue the existence of a minimizer in the presence of an external localizing potential (that vanishes at infinity) P.L. Lions developed his well-known Concentration Compactness Lemma [**Ls1984**]. Also with T. Cazenave he developed a technique for arguing the orbital stability of the standing waves for Pekar's nonlinear problem [**CL1982**]. A survey from the mathematical perspective is provided by V. Moroz and J. van Schaftingen [**MvS2017**]. Some of these points shall be elaborated further below where the mathematical issues related to the strong-coupling limit are discussed.

[14]Feynman later wrote in [**Fy1985**] "The shell game we play is technically called 'renormalization'. But no matter how clever the word, it is still what I would call a dippy process! Having to resort to such hocus-pocus has prevented us from proving that the theory of quantum electrodynamics is mathematically self-consistent. It's surprising that the theory still hasn't been proved self-consistent one way or the other by now; I suspect that renormalization is not mathematically legitimate."

[15]In [**Fr1985**] Fröhlich writes "[Meson theory] led to many applications in the field of nuclear forces including the prediction of a neutral meson. It also faced many difficulties including infinities of various types. In 1948 I decided that fields in solids offer a theory free of such difficulties. This led to the development of the so-called large polaron and of the phonon induced electron interaction which as is well known occupies a high amount of research up to this day."

| Material | $\alpha$ | Material | $\alpha$ |
|---|---|---|---|
| CdTe | 0.31 | KI | 2.5 |
| CdS | 0.52 | RbCl | 3.81 |
| ZnSe | 0.43 | RbI | 3.16 |
| AgBr | 1.6 | CsI | 3.67 |
| AgCl | 1.8 | TlBr | 2.55 |
| $CdF_2$ | 3.2 | GaAS | 0.068 |
| InSb | 0.02 | GaP | 0.201 |
| KCl | 3.5 | InAs | 0.052 |
| KBr | 3.05 | $SrTiO_3$ | 4.5 |

FIGURE 1.1.4. Tabulated above are the electron-phonon coupling parameters for various materials used in dielectrics. The coupling parameter $\alpha > 0$ was introduced in 1950 in the work of Fröhlich, Pelzer and Zienau [**FPZ1950**].

of which requires that the spatial extension of the polaron is much larger than the lattice spacing.[16] For this reason the 1950 model is also referred to as the *large* polaron.[17] Most importantly they have introduced a dimensionless parameter $\sqrt{\alpha}$ in front of the interaction term of the Hamiltonian with

$$\alpha = \frac{e^2}{2\hbar}\left(\frac{1}{\varepsilon_\infty} - \frac{1}{\varepsilon_s}\right)\left(\frac{2m}{\hbar\omega_L}\right)^{1/2}$$

determining the strength of the electron-phonon coupling. Above $e$ is the electron charge, $\hbar$ is Planck's constant, $m$ is the Bloch effective mass of the electron,[18] $\omega_L$ is the frequency of the longitudinal phonon modes, which as in Fröhlich's 1937 model [**Fr1937**] are assumed to all be equal, and $\varepsilon_\infty$ and $\varepsilon_0$ are the index of refraction and the static dielectric constant, respectively, of the particular crystal.[19]

[16]In NaCl the spatial extension of the polaron is $2.8 \times 10^{-7}$ cm whereas the lattice spacing is $5.6 \times 10^{-8}$ cm.
[17]In some materials such as $NaMnO_2$ this continuum approximation is no longer appropriate. For treating such cases T. Holstein has proposed in 1959 another polaron model known in the literature as the Holstein- or *small* polaron [**Hs1959**]. An excellent survey is provided by D. Emin in [**Em1987**] and [**Em2012**]. Moreover, the first rigorous treatment of the Holstein polaron with disorder is provided only recently by R. Mavi and J. Schenker in [**MS2018**], though the effect of disorder was studied previously also by F. Bronold and H. Fehske in [**BF2002**] and by O.R. Tozer and W. Barford in [**TB2014**]. It is an interesting open problem to understand the effect of disorder on bipolaron formation. Likewise, it remains to be seen how disorder influences the effective mass of the Holstein polaron.
[18]The Bloch effective mass is a central concept in band theory describing the mass of an electron moving in an ideal crystal with a periodic lattice structure. It is larger than the bare electron mass, but it does not account for the electron-phonon interaction. The Bloch effective mass should not be confused with the polaron effective mass, which is larger than the Bloch effective mass and is also material-dependent.
[19]It is worth noting that while $\alpha$ is analogous to the fine-structure constant $e^2/\hbar c \approx 1/137$ in Quantum Electrodynamics the quantities $\omega_L$, $\varepsilon_\infty$ and $\varepsilon_0$ are in fact material dependent.

In [**FPZ1950**] Fröhlich, Pelzer and Zienau have pointed out that Pekar's adiabatic treatment while certainly computationally convenient can in fact only be valid for strong coupling[20] $\alpha \gg 1$ cf. Fig. 1.1.4. The observation marks an important stage in the development of the polaron concept having inspired physicists to devise more suitable variational approaches for the weak and intermediate coupling regimes. The opposite limiting case $\alpha \ll 1$ (now the phonons are able to follow the electron) was also first considered in [**FPZ1950**] using a second-order perturbation theory under the assumption that no more than one phonon is excited by the electron at any given time,[21] and they have calculated the ground-state energy and effective mass to be

$$E_0 = -\alpha\hbar\omega_L \quad \text{and} \quad m^* = m/(1-\alpha/6) \quad \text{when} \quad \alpha \ll 1.$$

This should be compared with the respective expressions from Pekar's adiabatic treatment

$$E_0 \approx -0.108\alpha^2\hbar\omega_L \quad \text{and} \quad m^* = m(1+.02\alpha^4) \quad \text{when} \quad \alpha \gg 1.$$

In 1953 to do away with the artificial restriction $\alpha \ll 1$ in [**FPZ1950**] T.D Lee, F.E. Low and D. Pines have made an Ansatz in [**LLP1953**] for the ground-state wave function based on their feeling that there are no correlations between successively excited phonons.[22] Their calculations indeed agree with those in [**FPZ1950**] for $\alpha \ll 1$ but the validity of the variational approach in [**LLP1953**] rests on the fact that not too many phonons are excited in the first place (to neglect correlations). Since in this regime the number of excited phonons is $O(\alpha)$ the coupling parameter cannot be too large.[23] Subsequently Fröhlich in [**Fr1954**] compared the weak- and strong-coupling approaches of Lee-Low-Pines and Pekar: he found that they agreed at $\alpha \approx 10$ (but not smoothly!). There he advertised the need for an all-coupling theory with the hope that progress on the polaron problem can lead to the development of new techniques useful for addressing more fashionable problems in Quantum Field Theory and Solid State Physics such as Superconductivity. This in turn has motivated[24] R.P. Feynman in 1955 to use the path integral to develop an intermediate-coupling theory that is applicable to a wider range of coupling parameters [**Fy1955**]**.**

With the publication of the paper [**Fy1955**] Feynman has launched the polaron into the spotlight, and countless variational theories have been developed in the 1950s based on increasingly sophisticated modifications to his path integral technique. Indeed the vast majority of the current physics literature treats the polaron within the framework of Feynman's

[20]Pekar's Ansatz is based on a physical caricature that the phonons are too slow to follow the electron. This means the phonon frequency $\omega_L \ll 1$, which by definition of the electron-phonon coupling parameter means $\alpha \gg 1$. Moreover at strong-coupling the phonon cloud is very large–the number of phonons that are excited at any given time is $O(\alpha^2)$–making it very likely that there are correlations between successively excited phonons. These correlations make plausible the formation of a potential well around the electron leading to the self-trapping predicted by Landau in [**Ld1933**].

[21]This is known as the Tamm-Dancoff approximation in Quantum Field Theory. See also [**WP1965**]. This one-phonon approximation is only appropriate at sufficiently small coupling, since the phonon cloud is small.

[22]They use a variational technique introduced by S. Tomonaga in [**Ta1947**] for treating meson-theoretic problems.

[23]Another similar attempt has been made independently by M. Gurari in [**Gr1953**] where again the coupling parameter could not be too large.

[24]In [**Fr1954**] Fröhlich (vaguely) mentioned that developing an intermediate-coupling theory of the polaron could in fact be useful for understanding superconductivity. This is what seems to have enticed Feynman to consider the polaron: His letter to Fröhlich presenting his path integral approach ends with "What can we do to understand superconductivity?". See [**Hy2015**].

theory, considered since the mid-1950s as the most successful approach. Nevertheless to this day there does not exist–despite several attempts e.g. [**Ym1956**], [**Ym1982**], [**Ym1988**]–an equivalent Hamiltonian formulation of Feynman's path integral technique: one of the many outstanding idiosyncrasies afflicting Fröhlich's polaron! Furthermore at this point in the story it is worth reminding ourselves that all these variational theories provide only an *upper bound* of the true ground-state energy. Towards the end of the decade, however, a remarkable paper [**LY1958**] on the strongly coupled polaron has appeared: in Kyoto E.H. Lieb and K. Yamazaki[25] have arrived at a lower bound for the ground-state energy–differing from Pekar's upper bound by only a factor of three–by means of a *rigorously* controlled modification of the Hamiltonian rather than by making an Ansatz about the wave function. Moreover the argument in [**LY1958**] is quite simple, relying on a commutator estimate, and continues to play a central role in mathematical treatments of the strongly coupled polaron.

Meanwhile in the USSR criticisms[26] of Pekar's theory for addressing even the strong-coupling regime have been underway. The general consensus already in the 1950s has been that at strong coupling–and unlike in the weak and intermediate coupling regimes as discussed in [**FPZ1950**]–Pekar's adiabatic treatment seems to describe the ground-state energy and the effective mass rather accurately. Now the cause of contention was Pekar's Produkt Ansatz for the ground-state wave function. It should be recalled that Pekar's entire nonlinear theory was built on his use of a product wave function motivated by a suggestion of L.D. Landau about self-trapping of an electron in its own phonon cloud, and indeed the electronic wave function in his Ansatz–a minimizer of his nonlinear problem for the ground-state energy–is localized on a length scale of order $\alpha^{-1}$ whereas the corresponding Fröhlich Hamiltonian is translation invariant. The success of Pekar's theory when $\alpha \gg 1$ has led to the feeling that there is indeed a breaking of the translational symmetry at strong coupling i.e. the electron localizes itself in its own polarization well as predicted by Landau. But some physicists remained skeptical of Landau's speculation and viewed the breaking of translation symmetry in the strong-coupling regime as merely an artifact of Pekar's variational calculation. Starting as early as 1949 with the work of N.N. Bogoliubov and S.V. Tyablikov [**BT1949**] some physicists have set out to develop alternate strong-coupling variational theories that agree with Pekar's calculations of the ground-state energy and effective mass while preserving the translational symmetry [**Tv1951**], [**Gs1955**], [**Hr1955**], [**Ac1956**], [**Ta1961**].

By the late 1950s Pekar himself joined the ranks of the critics, and together with V.M. Buimistrov in [**BP1958**] he has restored the translational invariance to his previous adiabatic treatment by considering instead a "translational average" of his earlier product wave function, which it shall be recalled consists of a localized electronic wave function multiplied with a coherent state. Remarkably when $\alpha \gg 1$ the calculated values of the ground-state energy and effective mass from Buimistrov and Pekar's translation-invariant variational theory agree with those from Pekar's initial adiabatic treatment employing the Product Ansatz. The calculation in [**BP1958**] uses in an essential way the (almost) orthogonality when $\alpha \gg 1$ of

[25] Kazuo Yamazaki tried in [**Ym1956**] to develop Feynman's theory in terms of more pedestrian manipulations of the wave function and Hamiltonian. His later joint work at Kyoto with Elliott H. Lieb [**LY1958**] is partly motivated by same concerns. He pursued this program of "translating" Feynman's theory into a more direct operator-theoretic framework well into the 1980s [**Ym1982**], [**Ym1988**]. This philosophy has fully manifested itself in 1997 in the work of Lieb and L.E. Thomas [**LT1997**] to be discussed below.

[26] An excellent survey is provided by E.P. Gross [**Gs1975**] and by V.D. Lakhno in [**Lo2015**].

the different translates of the coherent state from Pekar's initial Ansatz. The translational-invariant approach in [**BP1958**] has been rediscovered independently three decades later by P. Nagy in [**Ny1989**] and more recently by Lieb and R. Seiringer [**LS2014**].

As explained by V.D. Lakhno in [**Lo2015**] not everyone was satisfied with the treatment in [**BP1958**] and some physicists have gone on to propose alternate translation-invariant theories for the strongly coupled Fröhlich polaron most notable among them being E.P. Gross who pursued this program well into the 1970s [**Gs1975**]. On the other hand the vast majority of the physicists still believed Landau's claims about self-trapping and many papers have been written with the sole purpose of calculating the critical electron-phonon coupling parameter at which the translation-invariant Fröhlich polaron exhibits a delocalization-localization transition. In fact it has taken three more decades to finally settle once and for all the debate about self-localization with B. Gerlach and H. Löwen proving in 1988 that the ground-state wave function of the translation-invariant Fröhlich Hamiltonian remains delocalized for all values of the electron-phonon coupling parameter $\alpha > 0$ [**GL1988**].

In 1980 using the large deviation techniques developed earlier by M.D. Donsker and S.R.S. Varadhan in [**DV1975**], [**DV1975-II**], [**DV1975-III**] and [**DV1976**] J. Adamowski, Gerlach and H. Leschke have argued formally that in the strong-coupling limit $\alpha \to \infty$ the ground-state energy *to leading order*[27] is described exactly by Pekar's nonlinear minimization problem [**AGH1980**]. A rigorous proof has been provided shortly thereafter by Donsker and Varadhan in [**DV1983**]. In 1997 a more pedestrian proof in the spirit of the argument in [**LY1958**] has been given in [**LT1997**] by Lieb and L.E. Thomas, who using rigorously controlled modifications of the Hamiltonian have arrived at a lower bound that agrees to leading order with Pekar's upper bound ($\approx -0.108\alpha^2\hbar\omega_L$). The main idea in [**LT1997**] is to instead consider while incurring an error of only $O\left(\alpha^{9/5}\right)$ a Hamiltonian describing an electron interacting with finitely many phonon modes. Then using the coherent state integral representation of creation and annihilation operators and just completing the square Lieb and Thomas have extracted the nonlinear energy functional from Pekar's minimization problem as a lower bound. Their technique is quite robust and has motivated the recent study of multipolaron systems [**AL2013**], [**BB2011**], [**GM2010**]. Most importantly it is central to R.L. Frank and L. Geisinger's analysis of the polaron in a strong magnetic field [**FG2015**] discussed in Section 1.2.

The mathematically rigorous work of Gerlach and Löwen [**GL1988**] closes an important chapter in the development of the polaron concept. The argument of Donsker and Varadhan [**DV1988**] on the other hand should be viewed as the beginning of a new chapter for the strongly coupled polaron–and one that is far from complete: It still remains to understand rigorously how well Pekar's nonlinear theory describes the ground-state wave function and the effective mass in the strong-coupling limit. To this end the recent work of Lieb and Seiringer [**LS2019**] demonstrates the divergence of the effective mass in the strong-coupling limit, but

[27] There have been attempts over the years to also calculate the subleading term of the ground-state energy in the strong-coupling regime describing the quantum fluctuation about the classical limit, Pekar's nonlinear theory. These quantum fluctuations contribute to keeping the ground state delocalized whereas the minimizers of Pekar's optimization problem for the ground-state energy are localized on a length scale $\alpha^{-1}$. In particular it has been suggested by G.R. Allcock that the subleading term is $\mathcal{O}\left(\alpha^{-2}\right)$ [**Ac1963**]. Allock's argument has been made rigorous recently by Rupert L. Frank and Robert Seiringer in [**FSr2019**]. (It should be emphasized that in [**FSr2019**] the polaron is restricted to a set of finite volume; essential to their argument is a result of D. Feliciangeli and R. Seiringer about the uniqueness of minimizers of the Pekar functional on the ball [**DF2019**].)

it is not clear whether the rate of divergence is $\alpha^4$ as calculated by Landau and Pekar in [**LP1948**] (and generally accepted in the physics community). Furthermore what place if any at all does the ground-state wave function–proved to be delocalized in [**GL1988**]–have in Pekar's local theory? Revisiting the paper [**BP1958**] by Buimistrov and Pekar it would be natural to conjecture–as did Nagy [**Ny1989**] and Lieb and Seiringer [**LS2014**]–that the delocalized ground-state wave function should be close to the "translational average" of Pekar's product wave function. This shall be discussed precisely using a Fiber decomposition of the translation-invariant Fröhlich Hamiltonian in Section 1.3.

Also in Section 1.3 is described an analogous problem addressing the strongly coupled polaron now bound in a Mexican hat-type potential that is scaled appropriately with the electron-phonon coupling parameter. The ground-state wave function is unique and therefore invariant under rotations. However it is shown that the minimizers of the corresponding Pekar problem are nonradial. Now–again looking for inspiration at the work [**BP1958**]–it would be natural to expect that the ground state is close to the rotational average of Pekar's wave functions. Under the assumption that the minimizers are unique up to rotation we confirm this expectation. Though this is certainly a contribution of the thesis it is not the main result.

The main concern of this thesis is polarons in strong magnetic fields. A non-relativistic Hydrogen atom in a strong magnetic field interacting with the quantized longitudinal optical modes of an ionic crystal is considered within the framework of Fröhlich's 1950 polaron model [**FPZ1950**]. Starting with Platzman's variational treatment in 1961 the polaron Hydrogenic atom has been of interest for describing an electron bound to a donor impurity in a semiconductor [**Pz1961**]. Its first rigorous examination, however, came much later in 1988 from Löwen, who disproved several longstanding claims about a self-trapping transition [**Lw1988a**].

A study of the polaron Hydrogenic atom in strong magnetic fields was initiated by Larsen in 1968 for interpreting cyclotron resonance measurements in InSb [**La1968**]. The model has since been considered in formal analogy to the Hydrogen atom in a magnetic field though the latter was understood rigorously again much later in 1981 by Avron et. al, who proved several properties including the non-degeneracy of the ground state [**AHS1981**]. Whether or not these Hydrogenic properties indeed persist when the coupling to a quantized field is turned on remains to be seen.

In any case polarons are the simplest Quantum Field Theory models, yet their most basic features such as the effective mass, ground-state energy and wave function cannot be evaluated explicitly. And while several successful theories have been proposed over the years to approximate the energy and effective mass of various polarons, they are built entirely on unjustified, even questionable, Ansätze for the wave function. The thesis provides for the first time an explicit description of the ground-state wave function of a polaron in an asymptotic regime namely in the strong magnetic field.

For the polaron Hydrogenic atom in a homogeneous magnetic field of strength $B$, it is shown that the ground-state electron density in the direction of the magnetic field converges as $B \to \infty$ to the square of a hyperbolic secant function–a sharp contrast to the Gaussian variational wave functions in the literature [**ZBK1996**], [**SPD1993**] & ref. therein. The explicit limiting function is realized as a density of the minimizer of a one-dimensional problem with a delta-function potential, which describes the second leading-order term of the ground-state energy in the limit $B \to \infty$.

In the direction of the magnetic field both the ground-state energy and wave function of a polaron Hydrogenic atom in a strong magnetic field are described by a one-dimensional model localized in a delta-function potential. In fact it was Kochetov et al. in **[KLS1992]** who have first derived–albeit formally–an effective one-dimensional theory of polarons in strong magnetic fields. Their arguments have been placed on a rigorous footing, at least for calculating the ground-state energy, only recently by Frank et. al in **[FG2015]**. The thesis now extends the description to the wave function. A one-dimensional description should extend also to the binding, dynamics and effective mass of polarons in strong magnetic fields and this shall be addressed in Section 1.4.

## 1.2. Model and Main Result

The model is defined by the Hamiltonian

$$\mathbb{H}(B) := H_B - \partial_3^2 - \beta\,|x|^{-1} + \mathcal{N} + \frac{\sqrt{\alpha}}{2\pi}\int_{\mathbb{R}^3}\left(\frac{a_k e^{ik\cdot x}}{|k|} + \frac{a_k^\dagger e^{-ik\cdot x}}{|k|}\right) dk \tag{1.2.1}$$

acting on the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^3)\otimes\mathcal{F}$ where $\mathcal{F} := \oplus_{n\geq 0}{}_s^n L^2(\mathbb{R}^3)$ is a symmetric phonon Fock space over $L^2(\mathbb{R}^3)$. The creation and annihilation operators for a phonon mode $a_k^\dagger$ and $a_k$ act on $\mathcal{F}$ and satisfy $[a_k, a_{k'}^\dagger] = \delta(k-k')$. The energy of the phonon field is described by the operator $\mathcal{N} = \int_{\mathbb{R}^3} a_k^\dagger a_k\, dk$. The kinetic energy of the electron is described by the operator $H_B - \partial_3^2$ acting on $L^2(\mathbb{R}^3)$, where $H_B = \sum_{j=1,2}\left(-i\partial_j + A_j(\mathbf{x})\right)^2$ is the two-dimensional Landau Hamiltonian with the magnetic vector potential $A\left(x_1,x_2,x_3\right) = \frac{B}{2}\left(-x_2,x_1,0\right)$ corresponding to a homogeneous magnetic field of strength $B>0$ in the $x_3$-direction; the transverse coordinates are denoted by $x_\perp = (x_1,x_2)$. Furthermore $\inf\operatorname{spec} H_B = B$. The parameters $\alpha\geq 0$, $\beta>0$ denote the strengths of the electron-phonon coupling and the localizing Coulomb potential. The ground-state energy is

$$E_0(B) := \inf\left\{\langle\Psi,\, \mathbb{H}(B)\Psi\rangle :\ \|\Psi\|_{\mathcal{H}} = 1,\ \Psi\in H_A^1\left(\mathbb{R}^3\right)\otimes\operatorname{dom}\left(\sqrt{\mathcal{N}}\right)\right\}, \tag{1.2.2}$$

where $H_A^1\left(\mathbb{R}^3\right)$ is the magnetic Sobolev space of order one with the vector potential given above. Since the Schrödinger operator $-i\nabla - \beta|x|^{-1}$ has a negative energy bound state in $L^2(\mathbb{R}^3)$, a ground state exists **[GLL2001]**; in fact the result applies equally well to an approximate ground state.

Unlike previous treatments here the arguments remain valid for all values of the parameters $\alpha\geq 0$, $\beta>0$. First the large $B$ asymptotics of the ground-state energy are derived. Since the pioneering work of Larsen the model has been considered only in the perturbative regime $\alpha\ll\beta$, and the ground-state energy $E_0(B)$ has been approximated as the Hydrogenic energy

$$E_H(B) := \inf\text{ spec } H_B - \partial_3^2 - \beta\,|x|^{-1} \tag{1.2.3}$$

with a supposedly small correction from the electron-phonon interaction. It was only in 1981 that the large $B$ asymptotics of the Hydrogenic energy were shown rigorously by Avron et. al **[AHS1981]**, who proved

$$E_H(B) = B - \frac{\beta^2}{4}\left(\ln B\right)^2 + \beta^2\ln B\ln\ln B + \mathcal{O}\left(\ln B\right)\ \text{ as } B\to\infty. \tag{1.2.4}$$

The first two terms in the expansion are just what one would expect heuristically. For large $B$ the electron is tightly bound in the transverse plane to the lowest Landau orbit while localized in the magnetic field direction by an effective Coulomb potential that behaves like a one-dimensional delta well of strength $\beta \ln B$. The electron motion is effectively one-dimensional, and the second leading-order term describes the energy of the electron confined along the magnetic field.

The above Hydrogenic heuristics still apply when a coupling to the phonon field is introduced i.e. $\alpha > 0$. Physically, for large $B$ the phonons cannot follow the electron's rapid motion in the transverse plane and so resign themselves to dressing its entire Landau orbit. The system effectively behaves like a strongly coupled one-dimensional polaron with interaction strength $\alpha \ln B$ again localized as above in the magnetic field direction by a delta well of strength $\beta \ln B$, i.e. in the effective model the electron-phonon interaction is now mediated by the magnetic field strength cf. [**KLS1992**]. In fact the effective potential and electron-phonon interaction energies scale the same way, contributing to the second leading-order term in the analogous large $B$ expansion of the polaron Hydrogenic energy.

THEOREM 1. *Let $E_0(B)$ be as defined in (1.2.2) above. Then*

$$E_0(B) = B + \mathfrak{e}_0 (\ln B)^2 + \mathcal{O}\left((\ln B)^{3/2}\right) \text{ as } B \to \infty, \tag{1.2.5}$$

*where*

$$\mathfrak{e}_0 := \inf\left\{ \int_{\mathbb{R}} |\varphi'|^2 \, dx - \frac{\alpha}{2} \int_{\mathbb{R}} |\varphi|^4 \, dx - \beta \, |\varphi(0)|^2 : \int_{\mathbb{R}} |\varphi|^2 \, dx = 1 \right\} \tag{1.2.6}$$

$$= -\frac{1}{48}\left(\alpha^2 + 6\alpha\beta + 12\beta^2\right). \tag{1.2.7}$$

Here the second leading-order term describes the dominant asymptotic behavior of the ground-state energy of the one-dimensional polaron confined along the magnetic field. It is evaluated explicitly by minimizing an effective nonlinear functional. Furthermore the mixing of the parameters $\alpha$ and $\beta$ in (1.2.7) indicates that for large $B$ the effect of the electron-phonon interaction is not perturbative.

The energy asymptotics for the case $\beta = 0$ was first proved by Frank et. al in [**FG2015**]. The proof of Theorem 1 follows mostly the argument in [**FG2015**] by arguing upper and lower bounds on $E_0(B)$. Their strategy with a trial product state is used to arrive at an upper bound. The strategy in [**FG2015**] for arguing a lower bound by reducing the problem to the lowest Landau level, however, requires two modifications. First, the proof here needs to accommodate the Coulomb potential, which does not commute with the projection onto the lowest Landau level. Furthermore a new idea is needed for extracting the delta-function from the Coulomb potential after projecting onto the lowest Landau level. This is accomplished by invoking the bathtub principle. After reducing to the lowest Landau level we follow [**FG2015**] and extract a one-dimensional Hamiltonian and apply the one-dimensional Lieb-Thomas proof in [**LT1997**] (see also [**Gh2012**]).

The upper bound is provided in Chapter 3 and the lower bound is provided in Chapter 4.

Frank and Geisinger's work makes rigorous an argument of Kochetov, Leschke and Smondyrev [**KLS1992**] that as $B \to \infty$ the (three-dimensional) polaron exposed to a homogenous magnetic field becomes "equivalent" to a one-dimensional polaron (without a magnetic field) with its electron-phonon coupling parameter multiplied by $\ln B$. Though this has finally been placed on a rigorous footing–at least for calculating the ground-state energy–it remains to be understood whether other essential features of the model (effective mass, binding, dynamics, etc.) also take on a one-dimensional description with large $B$. The contribution of this work is to extend the one-dimensional description to the wave function:

THEOREM 2. *Let $\Psi^{(B)} \in \mathcal{H}$ be a ground state of the Hamiltonian $\mathbb{H}(B)$. The one-dimensional minimization problem given in (1.2.6) above admits a unique minimizer*

$$\phi_0\left(x_3\right) = \frac{\alpha + 2\beta}{\sqrt{8\alpha}\cosh\left(\left(\frac{\alpha+2\beta}{4}\right)|x_3| + \tanh^{-1}\left(\frac{2\beta}{\alpha+2\beta}\right)\right)}, \tag{1.2.8}$$

*and for $W$ a sum of a bounded Borel measure on the real line and a $L^{\infty}(\mathbb{R})$ function,*

$$\lim_{B\to\infty} \frac{1}{(\ln B)} \int_{\mathbb{R}} W(x_3)\left(\int_{\mathbb{R}^2} \left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2 \left(x_\perp, \frac{x_3}{(\ln B)}\right) dx_\perp\right) dx_3$$
$$= \int_{\mathbb{R}} W(x_3)\left|\phi_0\left(x_3\right)\right|^2 dx_3.$$

Since $W$ can be taken to be a delta function, pointwise convergence follows. The above theorem also applies to any normalized state $\tilde{\Psi}^{(B)} \in \mathcal{H}$ satisfying

$$\left\langle \tilde{\Psi}^{(B)}, \mathbb{H}(B)\tilde{\Psi}^{(B)}\right\rangle = E_0(B) + \mathfrak{o}\left((\ln B)^2\right). \tag{1.2.9}$$

Finally, the scaling of the wave function is as expected since the electron is localized on a length scale $(\ln B)^{-1}$ in the direction of the magnetic field.

The limiting function $\phi_0$ in (1.2.8) is rather different from the Gaussian wave function suggested by Kartheuser et. al in **[ZBK1996]**. Furthermore, as $\alpha \to 0$, $\phi_0$ converges pointwise to the function $\sqrt{1/2}\exp(-|x_3|/2)$. This should raise some questions about the perturbative treatments ($\alpha \ll \beta$) in the physics literature, which always rely on a Born-Oppenheimer approximation and take the electron wave function to be a Gaussian. In fact, Devreese et. al have even claimed that as $B \to \infty$, the electron wave function "changes" from an exponential function to a Gaussian **[SPD1993]**.

The strategy for proving Theorem 2 is now described. To the Hamiltonian $\mathbb{H}(B)$ from (1.2.1) is added $\epsilon$ times a one-dimensional test potential, scaled appropriately, in the direction of the magnetic field. Denoting $E_\epsilon(B)$ to be the ground-state energy corresponding to the Hamiltonian

$$\mathbb{H}_\epsilon(B) := \mathbb{H}(B) - \epsilon\,(\ln B)^2\, W\left((\ln B)\, x_3\right), \tag{1.2.10}$$

it will follow from a straightforward modification of the proof of Theorem 1 that

$$\lim_{B\to\infty} \frac{E_\epsilon(B) - B}{(\ln B)^2} = \mathfrak{e}_\epsilon, \tag{1.2.11}$$

where

$$\mathfrak{e}_\epsilon = \inf_{\|\varphi\|_{L^2(\mathbb{R})}=1} \left\{\int_{\mathbb{R}} |\varphi'|^2\, dx - \frac{\alpha}{2}\int_{\mathbb{R}} |\varphi|^4\, dx - \beta\,|\varphi(0)|^2 - \epsilon\int_{\mathbb{R}} W(x)\,|\varphi|^2\, dx\right\}. \tag{1.2.12}$$

For $\Psi^{(B)}$ the ground state of the Hamiltonian $\mathbb{H}(B)$, by the variational principle and a change of variable,

$$
\begin{aligned}
E_\epsilon(B) &\leq \left\langle \Psi^{(B)}, \mathbb{H}_\epsilon(B)\Psi^{(B)} \right\rangle \\
&= E_0(B) - \epsilon\,(\ln B) \int_{\mathbb{R}} W\left(x_3\right) \left( \int_{\mathbb{R}^2} \left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2 \left(x_{\perp, \frac{x_3}{(\ln B)}}\right) dx_\perp \right) dx_3.
\end{aligned}
$$

Let $\epsilon > 0$. By subtraction and division,

$$
\frac{E_0(B) - E_\epsilon(B)}{\epsilon\,(\ln B)^2} \geq \frac{1}{(\ln B)} \int_{\mathbb{R}} W\left(x_3\right) \left( \int_{\mathbb{R}^2} \left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2 \left(x_{\perp, \frac{x_3}{(\ln B)}}\right) dx_\perp \right) dx_3.
$$

Taking the limit $B \to \infty$, by Theorem 1 and (1.2.11) ,

$$
\frac{\mathfrak{e}_0 - \mathfrak{e}_\epsilon}{\epsilon} \geq \limsup_{B\to\infty} \frac{1}{(\ln B)} \int_{\mathbb{R}} W\left(x_3\right) \left( \int_{\mathbb{R}^2} \left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2 \left(x_{\perp, \frac{x_3}{(\ln B)}}\right) dx_\perp \right) dx_3.
$$

For $\epsilon < 0$, the above inequality is merely reversed with the "limsup" replaced by "liminf" on the righthand side, which, by the way, does not depend on $\epsilon$.

Theorem 2 will follow if the limit on the left-hand side exists as $\epsilon \to 0$. Indeed, as it will be shown below, the one-dimensional minimization problem in (1.2.6) admits a *unique* minimizer. Armed with this fact, we show that the desired limit exists:

$$
\lim_{\epsilon\to 0} \frac{\mathfrak{e}_0 - \mathfrak{e}_\epsilon}{\epsilon} = \int_{\mathbb{R}} W\left(x\right) \left|\phi_0\left(x\right)\right|^2 dx.
$$

This important differentiation result is established in Chapter 2.

### 1.3. Mathematical Problems in the Strong-Coupling Limit

In this section I will discuss in more detail a problem going back to the very roots of polaron theory concerning the ground-state symmetry of a bound polaron. Consider the translation-invariant Fröhlich Hamiltonian

$$
H_\alpha = \mathbf{p}^2 + \int_{\mathbb{R}^3} a_k^\dagger a_k dk - \frac{\sqrt{\alpha}}{2\pi} \int_{\mathbb{R}^3} \left[ a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x} \right] \frac{dk}{|k|} \tag{1.3.1}
$$

acting on $\mathcal{H} := L^2(\mathbb{R}^3) \otimes \mathcal{F}$. By way of an (unjustified) Produkt-Ansatz Pekar concluded that when the coupling parameter $\alpha$ is large the ground-state wave function should be

$$
\Psi_\alpha = \alpha^{3/2}\varphi(\alpha x) \otimes \Phi_\alpha. \tag{1.3.2}
$$

Above, $\varphi \in L^2(\mathbb{R}^3)$ is the unique (modulo translations) minimizer for the Pekar minimization problem

$$
e_P := \inf_{\|\phi\|_2 = 1} \left\{ \int_{\mathbb{R}^3} |\nabla\phi|^2 dx - \frac{1}{2} \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\phi(x)|^2\,|\phi(y)|^2}{|x-y|} dx\,dy \right\}, \tag{1.3.3}
$$

and $\Phi_\alpha \in \mathcal{F}$ is a coherent state depending only on the phonon coordinates:

$$
\Phi_\alpha = \prod_k \exp\left( z_\alpha(k) a_k^\dagger - \overline{z_\alpha(k)} a_k \right) |0\rangle \tag{1.3.4}
$$

with the vacuum $|0\rangle \in \mathcal{F}$ and the phonon displacements

$$z_\alpha(k) = \frac{1}{\pi|k|}\sqrt{\frac{\alpha}{2}}\int_{\mathbb{R}^3} e^{-ik\cdot x}|\alpha^{3/2}\varphi(\alpha x)|^2 dx,$$

which depend on the electronic wave function.

Here we shall denote $E_\alpha$ to be the ground-state energy. Recall Pekar's wave function $\Psi_\alpha$ in (1.3.2) above. By the variational principle,

$$E_\alpha \leq \langle \Psi_\alpha, H_\alpha \Psi_\alpha\rangle_{L^2(\mathbb{R}^3)\otimes\mathcal{F}} = \alpha^2 e_P.$$

It is remarkable that Pekar's crude upper bound for the ground-state energy becomes exact (to the leading order) as $\alpha \to \infty$ :

$$\lim_{\alpha\to\infty}\frac{E_\alpha}{\alpha^2} = e_P. \tag{1.3.5}$$

Of course, with (1.3.5) it is natural to ask whether Pekar's wave function in (1.3.2) is indeed the true ground state of the translation-invariant polaron as $\alpha \to \infty$. Note, as $\alpha$ increases, Pekar's wave function becomes very localized. This led to the belief that the translation-invariant Fröhlich polaron exhibits a delocalization-localization transition, that at some some critical value of the electron-phonon interaction there will be a breaking of the translational symmetry. But it has been rigorously established by Gerlach and Löwen in the 1980s [**GL1988**] that the ground-state remains delocalized (it does not exist in $\mathcal{H}$) at all values of the electron-phonon interaction.

Gerlach and Löwen's seminal work presents us with a crisis: Does the (delocalized) ground state of the polaron really have a place in Pekar's nonlinear theory, which describes very well the ground-state energy (to the leading order in $\alpha$)? To frame this question precisely, as done by Lieb and Seiringer [**LS2014**] we will need a fiber decomposition of the Hamiltonian (1.3.1). Since the Hamiltonian $H_\alpha$ commutes with the total momentum $\mathcal{P} = p_x + P_f$ with

$$P_f := \int_{\mathbb{R}^3} k a_k^\dagger a_k dk$$

the field momentum, there is a well-known Fiber decomposition where $H_\alpha$ is restricted to states of fixed total momentum $P$, that is,

$$H_\alpha \equiv \int_{\mathbb{R}^3}^{\oplus} H_\alpha(P) dP$$

with the Fiber Hamiltonian

$$H_\alpha(P) := (P - P_f)^2 + \int_{\mathbb{R}^3} a_k^\dagger a_k dk - \frac{\sqrt{\alpha}}{(2\pi)}\int_{\mathbb{R}^3}\left[a_k + a_k^\dagger\right]\frac{dk}{|k|}$$

that acts on $\mathcal{F}$ alone.

We shall define the analogous ground-state energy

$$E_\alpha(P) = \mathrm{infspec} H_\alpha(P).$$

Provided that $|P|$ is small, there is a ground state $\Psi_\alpha^P \in \mathcal{F}$ [**LS2014**]. Restricting ourselves now to the $P = 0$ fiber, it follows that (see Proposition 4.1 in [**MS2007**])

$$\lim_{\alpha\to\infty}\frac{E_\alpha(0)}{\alpha^2} = e_P.$$

It is now a natural question to ask how, as $\alpha \to \infty$, the ground state $\Psi_\alpha^0$ of the $P = 0$ fiber Hamiltonian $H_\alpha(0)$ is related to the highly localized wave function of Pekar, given in (1.3.2)? Lieb and Seiringer conjecture that the Fiber ground state $\Psi_\alpha^0$ should be close to a "translational average" of Pekar's localized wave functions:

Conjecture. *For large $\alpha$, the ground state $\Psi_\alpha^0$ of the $P = 0$ fiber Hamiltonian $H_\alpha(0)$ is close to*

$$\hat{\varphi}(P_f)\Phi_\alpha := \alpha^{3/2} \int_{\mathbb{R}^3} e^{iP_f x} \varphi(\alpha x)\Phi_\alpha dx \in \mathcal{F}, \tag{1.3.6}$$

*where $\varphi$ and $\Phi_\alpha$ are the electronic wave function and coherent state in Pekar's wave function, given in (1.3.2) above.*

In fact, Nagy proposed this wave function in (1.3.6) decades earlier **[Ny1989]** to try to come to terms with the fact that Pekar's wave function is at odds with the translation-invariance of the system. He does a beautiful computation showing that

$$\lim_{\alpha\to\infty} \frac{\langle \hat{\varphi}(P_f)\Phi_\alpha, H_\alpha(0)\hat{\varphi}(P_f)\Phi_\alpha\rangle_{\mathcal{F}}}{\alpha^2} = e_p.$$

Essential to Nagy's computation is that different translates of Pekar's coherent state become orthogonal in the strong-coupling limit: for $x \neq y$,

$$\left\langle e^{iP_f x}\Phi_\alpha, e^{iP_f y}\Phi_\alpha \right\rangle_{\mathcal{F}} \to 0 \quad \text{as} \quad \alpha \to \infty.$$

In my previous work, I have been thinking about the convergence of the electron density. To address the above conjecture, it would be interesting to frame their question instead in terms of the convergence of (reduced) density matrix. It is also a curiosity whether the Quantum de Finetti theorem developed in **[LNR2014]** could be of use.

Now I shall describe an analogous problem–discussed in Chapter 5–with the Hamiltonian

$$H_\alpha(V) = \mathbf{p}^2 + \int a_{\mathbf{k}}^\dagger a_{\mathbf{k}} dk - \frac{\sqrt{\alpha}}{2\pi} \int_{\mathbb{R}^3} \left( \frac{a_k e^{ik\cdot x}}{|k|} + \frac{a_k^\dagger e^{-ik\cdot x}}{|k|} \right) dk + \alpha^2 V(\alpha x). \tag{1.3.7}$$

The potential needs to be scaled with the electron-phonon coupling parameter in order for its effect to survive in the strong-coupling limit. As already mentioned above, minimizing $\langle \Psi,\ H_\alpha \Psi\rangle$ over the more restrictive set of product wave functions of Pekar yields the following *upper bound* for the true ground state energy:

$$E_\alpha(V) \leq \inf \left\{ \langle \Psi,\ H_\alpha(V)\Psi\rangle_{\mathcal{F}\otimes L^2(\mathbb{R}^3)} \mid \|\Psi\|_{\mathcal{F}\otimes L^2(\mathbb{R}^3)} = 1 \text{ and } \Psi = |\phi\rangle \otimes |\zeta\rangle \right\} \tag{1.3.8}$$

$$= \alpha^2 e(V), \tag{1.3.9}$$

where

$e(V) :=$

$$\inf \left\{ \int_{\mathbb{R}^3} |\nabla\phi|^2 d\mathbf{x} - \frac{1}{2} \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\phi(\mathbf{x})|^2 |\phi(\mathbf{y})|^2}{|\mathbf{x}-\mathbf{y}|} d\mathbf{x}\, d\mathbf{y} - \int_{\mathbb{R}^3} V(x) |\phi(\mathbf{x})|^2 dx \mid \int_{\mathbb{R}^3} \phi(\mathbf{x})^2 d\mathbf{x} = 1 \right\}$$

and using the argument in **[LT1997]**

$$\lim_{\alpha\to\infty} \frac{E_\alpha(V)}{\alpha^2} = e(V). \tag{1.3.10}$$

Now consider the Mexican hat-type potential $V_R$ satisfying

$$V_R \in C_c^\infty\left(\mathbb{R}^3\right), \quad 0 \le V_R \le 1 \quad \text{and} \quad V_R(x) = \begin{cases} 0 & \text{when} \qquad |x| \le 1 \\ 1 & \text{when} \qquad 2 \le |x| \le R \\ 0 & \text{when} \qquad |x| \ge R+1 \end{cases}.$$

I consider the following natural question: Is it also the case that (the electron density of) a ground-state wave function also converges to a minimizer of the Pekar problem? For the Mexican hat-type potential $V_R$ given above, I show that this is not true by showcasing a discrepancy in rotational symmetry between the ground-state wave function and a minimizer of the Pekar problem.

It follows from standard techniques in Quantum Field Theory that the ground-state wave function $\Psi_\alpha^{V_R}$ is unique; as the potential $V_R$ is radial, the Hamiltonian $H_\alpha^{V_R}$ is rotation-invariant and it follows that the ground-state electron density $\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2(x)$ is also radial. However, I show that a minimizer of the Pekar problem above is not radial.

Theorem. *For $R$ large, the Pekar problem $e(V_R)$ admits only nonradial minimizers.*

This also implies that a minimizer of the Pekar problem is not unique. Furthermore the result presents a crisis (analogous to that facing the translation-invariant Fröhlich Hamiltonian) for the bound polaron. Though the Pekar minimization problem yields the exact ground-state energy in the strong-coupling limit, this discrepancy in symmetry means that there is no chance for the radial ground-state electron density to converge (pointwise or even in a weak sense) to a nonradial minimizer of the Pekar problem. Nevertheless, under some assumptions, I am able to iron out this inconsistency and show that, in the limit $\alpha \to \infty$, the wave function still has a place within Pekar's nonlinear theory:

Theorem. *Let $R$ be large enough so that $e(V_R)$ admits only nonradial minimizers. Let $\Psi_\alpha^{V_R} \in \mathcal{H}$ be the unique ground-state wave function. If the Pekar minimization problem admits a minimizer $u_{V_R}$ that is unique up to rotations, then denoting $\gamma$ to be the Haar measure on $SO(3)$,*

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi_\alpha^V\|_{\mathcal{F}}^2 \left(\frac{x}{\alpha}\right) W(x)\, dx = \int_{\mathbb{R}^3} \left[\int_{SO(3)} |u_{V_R}(\mathcal{R}x)|^2\, d\gamma(\mathcal{R})\right] W(x)\, dx \tag{1.3.11}$$

*for all $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.*

It should be emphasized that the rotational average itself is not a minimizer of the Pekar problem (which admits only non-radial minimizers). Moreover if the Pekar minimization problem does not admit a minimizer that is unique up to rotations, we conjecture that the ground-state electron density converges in the above sense to some convex combination of the rotational averages.

We now describe the strategy for proving the result about the rotational average. To the Hamiltonian $H_\alpha^{V_R}$ we add $\delta$ times the rotational average $\langle W\rangle$(x) of a test potential $W(x) \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ that is scaled appropriately:

$$H_\alpha\left(V_R\right) - \delta\alpha^2 \left\langle W\right\rangle (\alpha x), \tag{1.3.12}$$

where $\langle W\rangle = \int_{SO(3)} W(\mathcal{R}x)\,d\gamma(\mathcal{R})$. Denoting $E_\alpha\left(V_R + \delta\left\langle W\right\rangle\right)$ to be the ground-state energy of the Hamiltonian in (1.3.12), it follows from the variational principle that

$$\begin{aligned} E_\alpha\left(V_R + \delta\left\langle W\right\rangle\right) &\leq \left\langle \Psi_\alpha^{V_R},\, H_\alpha\left(V_R\right)\Psi_\alpha^{V_R}\right\rangle - \delta\alpha^2\int_{\mathbb{R}^3}\left\langle W\right\rangle(\alpha x)\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2(x)\;dx \\ &= E_\alpha\left(V_R\right) - \frac{\delta}{\alpha}\int_{\mathbb{R}^3}\left\langle W\right\rangle(x)\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\;dx. \end{aligned}$$

For $\delta > 0$, by subraction and division

$$\frac{E_\alpha\left(V_R + \delta\left\langle W\right\rangle\right) - E_\alpha\left(V_R\right)}{\delta\alpha^2} \leq -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\left\langle W\right\rangle(x)\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\;dx.$$

By (1.3.10),

$$\frac{e\left(V_R + \delta\left\langle W\right\rangle\right) - e\left(V_R\right)}{\delta} \leq \liminf_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\left\langle W\right\rangle(x)\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)dx \tag{1.3.13}$$

$$= \liminf_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3} W(x)\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)dx; \tag{1.3.14}$$

Above, (1.3.14) follows from Fubini's theorem and that $\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2(x)$ is a radial function.

When $\delta < 0$, the inequality in (1.3.13) is merely reversed with the "lim inf" replaced by "lim sup". Hence, the above theorem will follow if the map $\delta \mapsto e\left(V_R + \delta\left\langle W\right\rangle\right)$ is differentiable at $\delta = 0$. Because the minimization problem for the energy $e(V_R)$ does not admit a unique minimizer, the map $\delta \mapsto e(V_R + \delta J)$ cannot be differentiable for every $J \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. However, since (by assumption) the minimizers $u_{V_R}$ for the energy $e(V_R)$ are unique up to rotation, we will show that for all *radial* $Z \in L^{3/2}\left(\mathbb{R}^3\right) + L^\infty\left(\mathbb{R}^3\right)$,

$$\lim_{\delta\to 0}\frac{e\left(V_R + \delta Z\right) - e\left(V_R\right)}{\delta} = -\int_{\mathbb{R}^3} Z(x)\left|u_{V_R}(x)\right|^2 dx. \tag{1.3.15}$$

Choosing $Z(x) = \left\langle W\right\rangle(x)$ in (1.3.15), the above theorem about the rotational average then follows from Fubini's theorem.

### 1.4. Some Open Problems about Polarons in Strong Magnetic Fields

A one-dimensional description of a three-dimensional polarons in a strong magnetic fields should extend not only to the ground-state energy and wave function but also to other features of the model such as the effective mass, dynamics and binding cf. **[KLS1992]**. Here some problems about binding of polarons in strong magnetic fields are presented.

To understand bipolaron formation in strong magnetic fields–and to see rigorously that the presence of a magnetic field makes it easier for polarons to bind–it is necessary to come to grips with a one-dimensional problem with a delta interaction.

Here we will use somewhat different notation than above. The Hamiltonian for a single polaron in a homogeneous magnetic field of strength $B$ in the $x_3$-direction is given by

$$\mathbb{H}_{\alpha,B} = H_B - \partial_3^2 + \int_{\mathbb{R}^3} a_k^\dagger a_k dk + \frac{\sqrt{\alpha}}{(2\pi)^{3/2}}\int_{\mathbb{R}^3}\left[a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x}\right]\frac{dk}{|k|},$$

with

$$H_B = \left(-i\partial_1 + A_1(x)\right)^2 + \left(-i\partial_2 + A_2(x)\right)^2$$

and

$$A\left(x_1,x_2,x_3\right)=\frac{B}{2}\left(-x_2,x_1,0\right).$$

The ground-state energy of the model is given by

$$E_\alpha\left(B\right)=\inf_{\|\Psi\|_{L^2(\mathbb{R}^3)\otimes\mathcal{F}}}\left(\Psi,\,\mathbb{H}_{\alpha,B}\Psi\right). \tag{1.4.1}$$

The Hamiltonian for a bipolaron also in a homogeneous magnetic field of strength $B$ in the $x_3$- direction is given by

$$\begin{aligned}\mathbb{H}^{\mathrm{bip}}_{\alpha,B,U}=&\sum_{j=1}^{2}\left(H_{B,j}-\partial^2_{3,j}\right)+\frac{U}{|x_1-x_2|}+\int_{\mathbb{R}}a^\dagger_k a_k\,dk\\&+\frac{\sqrt{\alpha}}{(2\pi)^{3/2}}\sum_{j=1}^{2}\int_{\mathbb{R}^3}\left(\frac{a_k}{|k|}e^{ik\cdot x_j}+\frac{a^\dagger_k}{|k|}e^{-ik\cdot x_j}\right)dk\end{aligned} \tag{1.4.2}$$

with

$$H_{B,j}=\left(-i\partial_{1,j}+A_1(x)\right)^2+\left(-i\partial_{2,j}+A_2(x)\right)^2-\partial^2_{3,j}$$

the kinetic energy operator of the $j^{\mathrm{th}}$-electron, and the vector potential $A(x)$ as above. In the physical regime, $U\geq 2\alpha$. And the ground-state energy of the model is given by

$$E^{\mathrm{bip}}_{\alpha,U}(B)=\inf_{\|\Psi\|_{L^2(\mathbb{R}^6)\otimes\mathcal{F}}}\left(\Psi,\,\mathbb{H}^{\mathrm{bip}}_{\alpha,B,U}\Psi\right). \tag{1.4.3}$$

Next, we define the **binding energy**

$$\triangle E^{\mathrm{bip}}_{U,\alpha}\left(B\right)=2E_\alpha\left(B\right)-E^{\mathrm{bip}}_{\alpha,U}(B). \tag{1.4.4}$$

We note that $\triangle E^{\mathrm{bip}}_{U,\alpha}\left(B\right)\geq 0$, and if $\triangle E^{\mathrm{bip}}_{U,\alpha}\left(B\right)>0$ then **binding occurs**, i.e. there is bipolaron formation.

A line of inquiry that seems promising is the **existence of a critical Coulomb repulsion parameter for the absence of binding**:

**Question 3.** For each $B>0$ and $\alpha>0$ does there exist a finite constant $U_c(\alpha,B)>2\alpha$ such that

$$\triangle E^{\mathrm{bip}}_{U,\alpha}\left(B\right)=0\ \text{ for all } U\geq U_c\left(\alpha,\,B\right)? \tag{1.4.5}$$

When $B=0$ there is a rigorous argument for the absence of binding [**FLST2011**]:

Proposition. *For a given $\alpha>0$ there is a finite $U_c\left(\alpha,\,B\equiv 0\right)>2\alpha$ such that*

$$\triangle E^{bip}_{U,\alpha}\left(B\equiv 0\right)=0\ \textit{ for all }\ U>U_c\left(\alpha,B\equiv 0\right). \tag{1.4.6}$$

Moreover, not only is it suggested in the physical literature that there there exists a critical repulsion parameter $U_c(\alpha,B)$ but also that it is increasing in $B$ [**BD1996**]. In other words, the **presence of a magnetic field should make it easier for polarons to bind**. Since there is no rigorous proof of this, we state it as a conjecture:

Conjecture. *For a given $\alpha>0$, there exists a constant $U_c\left(\alpha,B\right)>2\alpha$ such that $\triangle E^{bip}_{U,\alpha}\left(B\right)=0$ for all $U\geq U_c(\alpha,B)$ and $U_c(\alpha,B)$ is increasing in $B$.*

I propose studying the above question about the critical Coulomb repulsion parameter in the presence of a strong magnetic field, which will require an analysis of the effective one-dimensional model.

It was shown in [**FG2015**] that the ground-state energy of single polaron in a homogeneous magnetic field is described by a one-dimensional problem:

PROPOSITION. *Let the ground state energy $E_\alpha(B)$ be as defined in (1.4.1) above. Then,*

$$\lim_{B\to\infty} \frac{E_\alpha(B) - B}{(\ln B)^2} = e_\alpha,$$

*where*

$$e_\alpha = \inf_{\|\varphi\|_{L^2(\mathbb{R})}=1} \left\{ \int_{\mathbb{R}} |\varphi'|^2\, dx - \frac{\alpha}{2} \int_{\mathbb{R}} |\varphi|^4\, dx \right\}.$$

This description should also be extended to the ground-state energy of the bipolaron in a strong magnetic field:

PROBLEM. Let the bipolaron energy $E^{\mathrm{bip}}_{U,\alpha}$ be as given in (1.4.3) above. Show that

$$\lim_{B\to\infty} \frac{E^{\mathrm{bip}}_{U,\alpha}(B) - 2B}{(\ln B)^2} = e^{\mathrm{bip}}_{U,\alpha}, \tag{1.4.7}$$

where

$$e^{\mathrm{bip}}_{U,\alpha} = \inf_{\psi\in L^2(\mathbb{R}^2)} \left\{ \sum_{j=1}^{2} \int_{\mathbb{R}^2} |\nabla_i \psi|^2\, dx\, dy + U \int_{\mathbb{R}} |\psi(x,x)|^2\, dx - \alpha \int_{\mathbb{R}} (\rho_\psi(x))^2\, dx \right\}$$

and

$$\rho_\psi(x) = \int_{\mathbb{R}} |\psi(x,z)|^2 dz + \int_{\mathbb{R}} |\psi(z,x)|^2 dz.$$

We can analogously define the binding energy for this **one-dimensional** model:

$$\triangle e^{\mathrm{bip}}_{U,\alpha} = 2e_\alpha - e^{\mathrm{bip}}_{U,\alpha}.$$

Clearly, understanding (the absence of) binding in strong magnetic fields requires understanding (the absence of) binding for corresponding nonlinear one-dimensional model:

**Question 5.** For each $\alpha > 0$ does there exist a constant $U_c^{1\mathcal{D}}(\alpha)$ such that $\triangle e^{\mathrm{bip}}_{U,\alpha} = 0$ for all $U > U_c^{1\mathcal{D}}(\alpha)$?

The next questions are predicated on successfully showing the existence of the critical paramters $U_c(\alpha, B)$ and $U_c^{1\mathcal{D}}(\alpha)$ in Question 3 and Question 5 above. And these, in my opinion, are the most interesting questions:

**Question 6.** What is the relationship between $U_c(\alpha, B)$ and $U_c^{1\mathcal{D}}(\alpha)$ as $B \to \infty$ (for fixed $\alpha$)?

Now, let $U_c(\alpha, B \equiv 0)$ be the critical repulsion parameter in the absence of the magnetic field. Recall that such a parameter was shown to exist in [**FLST2011**]. Then:

**Question 7.** Let $\alpha > 0$. Is $U_c(\alpha, B \equiv 0) < U_c^{1\mathcal{D}}(\alpha)$?

Here is the point: If we (1) successfully argue the existence of a critical repulsion parameter $U_c(\alpha, B)$ for all $B$ sufficiently large (see Question 3), (2) show that the ground-state energy of the magneto-bipolaron is given by a one-dimensional minimization problem (see (1.4.7) above), (3) successfully argue the existence of a critical parameter $U_c^{1\mathcal{D}}(\alpha)$ (see Question 5) and (4) show that the answer to Question 7 is "Yes", then we will make rigorous the hueristic argument of Brosens and Devreese that the presence of a strong magnetic field enhances bipolaron formation (see "Conjecture" above).

CHAPTER 2

# Differentiating the One-Dimensional Energy

The goal of the chapter is to establish the crucial differentiability result for the one-dimensional energy, given as Theorem 6, which relies on two important properties of the minimization problem. First the minimizer needs to unique. The uniqueness, which is given in Lemma 4, follows from solving the corresponding Euler-Lagrange equation. Second a compactness property, given in Theorem 3, for the minimizing sequences must be established.

The one-dimensional minimization problem for the energy $\mathfrak{e}_{0}$ in (1.2.6) shall be denoted

$$\mathfrak{e}_{0} := \inf_{\|\varphi\|_2=1} \mathcal{E}_{0}\left(\varphi\right)$$

where

$$\mathcal{E}_{0}\left(\varphi\right) := \int_{\mathbb{R}} \left|\varphi'\right|^2 dx - \frac{\alpha}{2}\int_{\mathbb{R}} \left|\varphi\right|^4 dx - \beta\left|\varphi(0)\right|^2. \tag{2.0.1}$$

THEOREM 3. *If a sequence $\{\psi_{n}\}_{n=1}^{\infty}$, $\|\psi_{n}\|_2 = 1$ satisfies $\lim_{n\to\infty} \mathcal{E}_{0}\left(\psi_{n}\right) = \mathfrak{e}_{0}$ with the functional $\mathcal{E}_{0}$ as given in (2.0.1), then there exists a subsequence $\{\psi_{n_k}\}_{k=1}^{\infty}$ and some $\psi \in H^1\left(\mathbb{R}\right)$ such that $\|\psi\|_2 = 1$, $\mathcal{E}_{0}\left(\psi\right) = \mathfrak{e}_{0}$ and $\|\psi_{n_k} - \psi\|_{H^1} \to 0$ as $k \to \infty$.*

PROOF. It follows from Hölder's inequality, the Sobolev inequality and completion of the square that for all $\varphi \in H^1\left(\mathbb{R}\right)$

$$\mathcal{E}_{0}\left(\varphi\right) \geq \frac{3}{4}\|\varphi'\|_2^2 - \|\varphi\|_2^2\left(\frac{\alpha}{2}\|\varphi\|_2^2 + \beta\right)^2.$$

Furthermore since $\psi_{n}$ is a minimizing sequence, $\mathcal{E}_{0}\left(\psi_{n}\right) < \mathfrak{e}_{0}+1$ for $n$ large. Then $\|\psi_{n}\|_{H^1} < C$ and there exists a subsequence $\{\psi_{n_k}\}_{k=1}^{\infty}$ and some $\psi \in H^1\left(\mathbb{R}\right)$ such that $\psi_{n_k}$ converges to $\psi$ weakly in $H^1\left(\mathbb{R}\right)$.

**Step 1** (Compactness). It shall be argued that the subsequence $\{\psi_{n_k}\}_{k=1}^{\infty}$ satisfies

$$\forall\delta > 0,\ \exists R < \infty \ \text{ s.t. } \ \|\psi_{n_k}\|^2_{L^2(\{|x|<R\})} > 1 - \delta. \tag{2.0.2}$$

Essential to the argument is the binding inequality $\mathfrak{e}_{0} < \mathfrak{e}_{T}$ where $\mathfrak{e}_{T} := \inf_{\|\varphi\|_2=1} \mathcal{E}_{T}\left(\varphi\right)$ with $\mathcal{E}_{T}\left(\varphi\right) := \int_{\mathbb{R}} \left|\varphi'\right|^2 dx - (\alpha/2)\int_{\mathbb{R}} \left|\varphi\right|^4 dx$ is the translation-invariant problem admitting a symmetric decreasing minimizer $\phi_{T}$ [**FG2015**]. Indeed

$$\mathfrak{e}_{0} \leq \mathcal{E}_{0}\left(\phi_{T}\right) = \mathcal{E}_{T}\left(\phi_{T}\right) - \beta\phi_{T}^2(0) = \mathfrak{e}_{T} - \beta\phi_{T}^2(0) < \mathfrak{e}_{T}.$$

Moreover it should be noted

$$\mathcal{E}_{0}\left(\varphi\right) \geq \mathfrak{e}_{0}\left\|\varphi\right\|_2^2 \quad \text{and} \quad \mathcal{E}_{T}\left(\varphi\right) \geq \mathfrak{e}_{T}\left\|\varphi\right\|_2^2 \quad \text{when} \quad \|\varphi\|_2 \leq 1. \tag{2.0.3}$$

Also a quadratic partition of unity is chosen, $\chi^2 + \tilde{\chi}^2 \equiv 1$, where $0 \leq \chi \leq 1$ is a smooth function with $\chi(x) = 1$ when $|x| < 1/2$ and $\chi(x) = 0$ when $|x| > 1$. Denoting $\chi_{R} := \chi\left(R^{-1}\cdot\right)$ it follows from (2.0.3) that

$$
\begin{aligned}
\mathcal{E}_0(\psi_{n_k}) = & \mathcal{E}_0(\chi_R\psi_{n_k}) + \mathcal{E}_T(\tilde{\chi}_R\psi_{n_k}) \\
& - 2\int_{\mathbb{R}} \chi_R^2\tilde{\chi}_R^2 |\psi_{n_k}|^4\, dx - \int_{\mathbb{R}} |\psi_{n_k}|^2 \left(|\chi_R'|^2 + |\tilde{\chi}_R'|^2\right) dx \\
\geq & (\mathfrak{e}_0 - \mathfrak{e}_T)\|\chi_R\psi_{n_k}\|_2^2 + \mathfrak{e}_T \\
& - 2\int_{\mathbb{R}} \chi_R^2\tilde{\chi}_R^2 |\psi_{n_k}|^4\, dx - \int_{\mathbb{R}} |\psi_{n_k}|^2 \left(|\chi_R'|^2 + |\tilde{\chi}_R'|^2\right) dx.
\end{aligned}
\tag{2.0.4}
$$

Since $\chi, \tilde{\chi}$ have bounded derivatives

$$
\int_{\mathbb{R}} |\psi_{n_k}|^2 \left(|\chi_R'|^2 + |\tilde{\chi}_R'|^2\right) dx < CR^{-2}
$$

for some $C > 0$. Furthermore denoting $D_R := \{R/2 \leq |x| \leq R\}$

$$
\int_{\mathbb{R}} \chi_R^2\tilde{\chi}_R^2 |\psi_{n_k}|^4\, dx \leq \|\psi_{n_k}\|_{L^4(D_R)}^4,
$$

and $\|\psi_{n_k}\|_{L^4(D_R)}^4 \longrightarrow \|\psi\|_{L^4(D_R)}^4$ by Rellich-Kondrashov, so the first term in (2.0.4) can also be made arbitrarily small with $R$ chosen to be large enough uniformly in $k$. Hence for any $\delta > 0$ there is some $R$ such that for all $k$

$$
\mathcal{E}_0(\psi_{n_k}) \geq (\mathfrak{e}_0 - \mathfrak{e}_T)\|\chi_R\psi_{n_k}\|_2^2 + \mathfrak{e}_T - \delta(\mathfrak{e}_T - \mathfrak{e}_0)/2. \tag{2.0.5}
$$

Since $\{\psi_{n_k}\}_{k=1}^{\infty}$ is a minimizing sequence for $\mathfrak{e}_0$, for $k$ large

$$
\mathcal{E}_0(\psi_{n_k}) \leq \mathfrak{e}_0 + \delta(\mathfrak{e}_T - \mathfrak{e}_0)/2. \tag{2.0.6}
$$

Compactness now follows from (2.0.5) and (2.0.6).

**Step 2** (Weak Limit is a Minimizer). By Rellich-Kondrashov and the compactness property in (2.0.2)

$$
\|\psi_{n_k} - \psi\|_2 \to 0 \quad \text{and} \quad \|\psi\|_2 = 1. \tag{2.0.7}
$$

Since $\|\psi_n\|_{H^1} < C$ by Sobolev and Hölder's inequalities

$$
\int_{\mathbb{R}} \left(|\psi_{n_k}|^4 - |\psi|^4\right) dx \leq C\|\psi_{n_k} - \psi\|_2 \longrightarrow 0.
$$

Furthermore by Theorem 8.6 in [**LL2001**] $\psi_{n_k}(0) \to \psi(0)$, so

$$
\frac{\alpha}{2}\int_{\mathbb{R}} |\psi_{n_k}|^4 dx + \beta|\psi_{n_k}(0)|^2 \to \frac{\alpha}{2}\int_{\mathbb{R}} |\psi|^4\, dx + \beta\,|\psi(0)|^2. \tag{2.0.8}
$$

Then since $\liminf_{k\to\infty} \|\psi_{n_k}'\|_2 \geq \|\psi'\|_2$,

$$
\mathfrak{e}_0 = \lim_{k\to\infty} \mathcal{E}_0(\psi_{n_k}) \geq \mathcal{E}_0(\psi) \geq \mathfrak{e}_0
$$

and $\mathcal{E}_0(\psi) = \mathfrak{e}_0$.

**Step 3** (Convergence in $H^1(\mathbb{R})$). From (2.0.8)

$$\begin{aligned}\lim_{k\to\infty}\|\psi'_{n_k}\|_2^2 &= \lim_{k\to\infty}\left(\mathcal{E}_0(\psi_{n_k})+\frac{\alpha}{2}\|\psi_{n_k}\|_4^4+\beta|\psi_{n_k}(0)|^2\right)\\ &= \mathfrak{e}_0+\frac{\alpha}{2}\|\psi\|_4^4+\beta|\psi(0)|^2\\ &= \|\psi'\|_2^2\end{aligned}$$

and since $\psi_{n_k} \rightharpoonup \psi$ in $H^1$, $\|\psi'_{n_k}-\psi'\|_2 \to 0$. Strong convergence in $H^1$ now follows from (2.0.7).

□

LEMMA 4. *The minimization problem in (1.2.6) for the energy $\mathfrak{e}_0$ admits a unique minimizer*

$$\phi_0(x)=\frac{\alpha+2\beta}{\sqrt{8\alpha}\cosh\left(\left(\frac{\alpha+2\beta}{4}\right)|x|+\tanh^{-1}\left(\frac{2\beta}{\alpha+2\beta}\right)\right)}$$

*and*

$$\mathfrak{e}_0=-\frac{1}{48}\left(\alpha^2+6\alpha\beta+12\beta^2\right).$$

PROOF. The existence of a minimizer follows from Theorem 3. Every minimizer is a nonnegative, $C^2(\mathbb{R}\setminus\{0\})$ function in $H^1(\mathbb{R})$ that solves the Euler-Lagrange equation $-\psi''-2\alpha\psi^3-\beta\delta(x)\psi=-\lambda\psi$ for some $\lambda$ where

$$-\lambda=\mathfrak{e}_0-\frac{\alpha}{2}\int_{\mathbb{R}}\psi^4dx<0. \tag{2.0.9}$$

Or equivalently it must solve

$$-\psi''-\alpha\psi^3=-\lambda\psi \quad \text{for } |x|>0 \tag{2.0.10}$$

and satisfy the boundary condition

$$\lim_{\epsilon\to0^+}\left[\psi'(-\epsilon)-\psi'(\epsilon)\right]=\beta\psi(0). \tag{2.0.11}$$

The first integral of (2.0.10) is

$$(\psi')^2=-\frac{\alpha}{2}\psi^4+\lambda\psi^2 \quad \text{for } |x|>0. \tag{2.0.12}$$

Any nonnegative, $C^2(\mathbb{R}\setminus\{0\})$ solution of (2.0.12) in $H^1(\mathbb{R})$ satisfying the boundary condition in (2.0.11) must be of the form

$$\psi=\sqrt{\frac{2\lambda}{\alpha}}\frac{1}{\cosh\left(\sqrt{\lambda}\left(|x|-\tau\right)\right)} \tag{2.0.13}$$

for some $\tau$ cf. [Fr]. The boundary condition and that $\|\psi\|_2=1$ require respectively

$$\tanh\left(\tau\sqrt{\lambda}\right)=-\frac{\beta}{2\sqrt{\lambda}} \quad \text{and} \quad \frac{\alpha}{4\sqrt{\lambda}}=1+\tanh\left(\tau\sqrt{\lambda}\right).$$

Any minimizer must therefore be of the form given in (2.0.13) with

$$\lambda=\left(\frac{\alpha+2\beta}{4}\right)^2 \quad \text{and} \quad \tau=-\frac{4}{\alpha+2\beta}\tanh^{-1}\left(\frac{2\beta}{\alpha+2\beta}\right)$$

and hence is unique. The explicit calculation of $\mathfrak{e}_0$ now follows from (2.0.9).

$\square$

LEMMA 5. *Every minimizing sequence for the energy* $\mathfrak{e}_0$ *converges in* $H^1(\mathbb{R})$ *to the unique minimizer* $\phi_0$.

PROOF. It is shown in Theorem 3 that every minimizing sequence has a subsequence converging in $H^1(\mathbb{R})$ to some minimizer. Since the minimizer is unique, the entire sequence converges.

$\square$

THEOREM 6. *Let* $W$ *be a sum of a bounded Borel measure on the real line and a* $L^\infty(\mathbb{R})$ *function. For* $\epsilon$ *a real parameter consider the perturbed one-dimensional energy*

$$\mathfrak{e}_\epsilon := \inf_{\|\varphi\|_2=1} \mathcal{E}_\epsilon(\varphi)$$

*where*

$$\mathcal{E}_\epsilon(\varphi) := \mathcal{E}_0(\varphi) - \epsilon \int_{\mathbb{R}} W(x) |\varphi|^2 \, dx$$

*with the functional* $\mathcal{E}_0$ *as given in (2.0.1). Then the map* $\epsilon \mapsto \mathfrak{e}_\epsilon$ *is differentiable at* $\epsilon = 0$ *and*

$$\left.\frac{d}{d\epsilon}\right|_{\epsilon=0} \mathfrak{e}_\epsilon = -\int_{\mathbb{R}} W(x) |\phi_0|^2 \, dx$$

*with* $\phi_0$ *the unique minimizer for the energy* $\mathfrak{e}_0$.

PROOF. Writing $W = \mu + \omega$ where $\mu$ is a signed, bounded measure on the real line and $\omega \in L^\infty(\mathbb{R})$, it follows from Hölder's inequality, the Sobolev inequality and completion of the square that for $\varphi \in H^1(\mathbb{R})$

$$\begin{aligned}\mathcal{E}_\epsilon(\varphi) &\geq \|\varphi'\|_2^2 - \|\varphi\|_\infty^2 \left(\frac{\alpha}{2}\|\varphi\|_2^2 + |\epsilon|\,|\mu|(\mathbb{R}) + \beta\right) - |\epsilon|\,\|\omega\|_\infty \|\varphi\|_2^2 \\ &\geq \frac{3}{4}\|\varphi'\|_2^2 - \|\varphi\|_2^2 \left(\frac{\alpha}{2}\|\varphi\|_2^2 + |\epsilon|\,|\mu|(\mathbb{R}) + \beta\right)^2 - |\epsilon|\,\|\omega\|_\infty \|\varphi\|_2^2. \end{aligned} \tag{2.0.14}$$

Hence $\mathfrak{e}_\epsilon > -\infty$, and for each $\epsilon$ there is a $\phi_\epsilon \in H^1(\mathbb{R})$ satisfying

$$\mathcal{E}_\epsilon(\phi_\epsilon) \leq \mathfrak{e}_\epsilon + \epsilon^2 \text{ and } \|\phi_\epsilon\|_2 = 1. \tag{2.0.15}$$

By the variational principle

$$\begin{aligned}\mathfrak{e}_0 \leq \mathcal{E}_0(\phi_\epsilon) &= \mathcal{E}_\epsilon(\phi_\epsilon) + \epsilon \int_{\mathbb{R}} W(x) |\phi_\epsilon|^2 \, dx \\ &\leq \mathfrak{e}_\epsilon + \epsilon^2 + \epsilon \int_{\mathbb{R}} W(x) |\phi_\epsilon|^2 \, dx\end{aligned}$$

and

$$\mathfrak{e}_\epsilon \leq \mathcal{E}_\epsilon(\phi_0) = \mathfrak{e}_0 - \epsilon \int_{\mathbb{R}} W(x) |\phi_0|^2 \, dx.$$

Then for $\epsilon > 0$

$$-\int_{\mathbb{R}} W(x) |\phi_\epsilon|^2 \, dx - \epsilon \leq \frac{\mathfrak{e}_\epsilon - \mathfrak{e}_0}{\epsilon} \leq -\int_{\mathbb{R}} W(x) |\phi_0|^2 \, dx, \tag{2.0.16}$$

and for $\epsilon < 0$ the inequalities in (2.0.16) are reversed. It therefore suffices to show for any sequence $\{\epsilon_n\}_{n=1}^{\infty}$, $|\epsilon_n| > 0$ and $\epsilon_n \to 0$ that

$$\lim_{n\to\infty} \int_{\mathbb{R}} W(x) \left|\phi_{\epsilon_n}\right|^2 dx = \int_{\mathbb{R}} W(x) \left|\phi_0\right|^2 dx. \tag{2.0.17}$$

Since $\mathfrak{e}_\epsilon > -\infty$, the concave map $\epsilon \mapsto \mathfrak{e}_\epsilon$ is continuous and $\mathfrak{e}_{\epsilon_n} < C$ for all $n$. It follows from (2.0.14), the Sobolev inequality and (2.0.15) that $\|\phi_{\epsilon_n}\|_\infty < C$ . Thus

$$\lim_{n\to\infty} \epsilon_n \int_{\mathbb{R}} W(x) \left|\phi_{\epsilon_n}\right|^2 dx = 0,$$

$$\begin{aligned} \mathfrak{e}_0 = \lim_{n\to\infty} \mathfrak{e}_{\epsilon_n} &\geq \limsup_{n\to\infty} \left( \mathcal{E}_0\left(\phi_{\epsilon_n}\right) - \epsilon_n \int_{\mathbb{R}} W(x) \left|\phi_{\epsilon_n}\right|^2 dx - \epsilon_n^2 \right) \\ &= \limsup_{n\to\infty} \mathcal{E}_0\left(\phi_{\epsilon_n}\right) \end{aligned}$$

and $\left\{\phi_{\epsilon_n}\right\}_{n=1}^{\infty}$ is a minimizing sequence for $\mathfrak{e}_0$. By Lemma 5 $\phi_{\epsilon_n}$ converges in $H^1(\mathbb{R})$ to $\phi_0$, and by Theorem 8.6 in [**LL2001**] $\phi_{\epsilon_n}$ converges also pointwise uniformly to $\phi_0$ on bounded sets. The convergence in (2.0.17) now follows.

□

CHAPTER 3

# Upper Bound for the Ground-State Energy

THEOREM 7. *There is a constant $C > 0$ such that for $B > 1$*

$$E_0(B) \leq B + \mathfrak{e}_0 (\ln B)^2 - 4\mathfrak{e}_0 \ln B \ln\ln B + C \ln B.$$

We first employ the *Pekar Ansatz*: that the ground state has the product form $\varphi(x)\Phi$, where $\varphi(x)$ is an electronic wave function and $\Phi \in \mathcal{F}$ is a coherent state depending only on the phonon coordinates,

$$\Phi = \prod_k \exp\left(z(k)a_k^\dagger - \overline{z(k)}a_k\right)|0\rangle$$

with the vacuum $|0\rangle \in \mathcal{F}$ and the phonon displacements $z(k) \in L^2(\mathbb{R}^3)$, to be determined variationally. In particular, a coherent state is an eigenstate of the annihlation operator, $a_k\Phi = z(k)\Phi$. Minimizing the quantity $\langle\Psi, \mathbb{H}(B)\Psi\rangle$ over the (more restrictive) set of these product wave functions and completing the square, one determines that

$$z(k) = -\frac{\sqrt{\alpha}}{2\pi\,|k|}\int_{\mathbb{R}^3} e^{-ik\cdot x}\,|\varphi(x)|^2\,dx \tag{3.0.1}$$

and arrives at an *upper bound* for the ground-state energy:

$$\begin{aligned} E_0(B) &\leq \inf\left\{\left(\Psi, \left(\mathbb{H}_{\alpha,B} - \beta|x|^{-1}\right)\Psi\right) \mid \|\Psi\| = 1 \text{ and } \Psi = \varphi(x)\Phi\right\} \\ &= \inf_{\|\varphi\|_{L^2(\mathbb{R}^3)}=1} \mathcal{P}(\varphi) \end{aligned} \tag{3.0.2}$$

with the magnetic Pekar functional

$$\mathcal{P}(\varphi) := \\ \left\langle\varphi, \left(H_B - \partial_3^2\right)\varphi\right\rangle_{L^2(\mathbb{R}^3)} - \frac{\alpha}{2}\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}\,dx\,dy - \beta\int_{\mathbb{R}^3}\frac{|\varphi(x)|^2}{|x|}\,dx.$$

The heuristic appeal of the Ansatz–at least with strong magnetic fields–is as follows: Since the electron's cyclotron frequency (in the transverse plane) increases with $B$, the phonons cannot follow the rapidly moving electron in a strong magnetic field and are therefore only sensitive to the "mean" electron density $\varphi^2(x)$. This is precisely reflected in (3.0.1), where the phonon displacements do not depend on the instantaneous position of the electron.

Next, we recall for the two-dimensional Landau Hamiltonian that $\operatorname{infspec} H_B = B$. By restricting to the Lowest Landau state (in the zero angular momentum sector)

$$\gamma_B(x_\perp) := \sqrt{\frac{B}{2\pi}}\exp\left(-\frac{B}{4}|x_\perp|^2\right), \text{ where } \left(\gamma_B, H_B\gamma_B\right)_{L^2(\mathbb{R}^2)} = B,$$

we obtain yet another upper bound now on the Pekar minimization problem in (3.0.2): for $\phi \in H^1(\mathbb{R})$ with $\|\phi\|_{L^2(\mathbb{R})} = 1$

$$\inf_{\|\varphi\|_{L^2(\mathbb{R}^3)}=1} \mathcal{P}(\varphi) \leq \mathcal{P}\left(\gamma_B(x_\perp)\,\phi(x_3)\right).$$

It follows from an elementary computation

$$V_{\mathcal{U}}^B(x_3) := \int_{\mathbb{R}^2} \frac{|\gamma_B(x_\perp)|^2}{\sqrt{|x_\perp|^2 + x_3^2}} dx_\perp = \int_0^\infty \frac{e^{-u}}{\sqrt{x_3^2 + u/B}}\, du. \tag{3.0.3}$$

Similarly, since $|x_\perp|^2 + |y_\perp|^2 = \frac{|x_\perp - y_\perp|^2}{2} + \frac{|x_\perp + y_\perp|^2}{2}$, we have

$$\int_{\mathbb{R}^2}\int_{\mathbb{R}^2} \frac{|\gamma_B(x_\perp)|^2\,|\gamma_B(y_\perp)|^2}{\sqrt{|x_\perp - y_\perp|^2 + (x_3 - y_3)^2}} dx_\perp dy_\perp = \frac{1}{\sqrt{2}} V_{\mathcal{U}}^B\left(\frac{x_3 - y_3}{\sqrt{2}}\right).$$

Then, for any $\phi \in H^1(\mathbb{R})$

$$\begin{aligned}
&\mathcal{P}\left(\gamma_B(x_\perp)\,\phi(x_3)\right)\\
&= B + \int_{\mathbb{R}} |\phi'|\, dx_3 - \frac{\alpha}{2\sqrt{2}} \int\int_{\mathbb{R}\times\mathbb{R}} |\phi(x_3)|^2\, V_{\mathcal{U}}^B\left(\frac{x_3 - y_3}{\sqrt{2}}\right) |\phi(y_3)|^2\, dx_3 dy_3\\
&- \beta \int_{\mathbb{R}} |\phi(x_3)|^2\, V_{\mathcal{U}}^B(x_3)\, dx_3.
\end{aligned}$$

We will require the following estimate on the effective Coulomb potential $V_{\mathcal{U}}^B$.

Lemma 8. *For any $L > 0$ and $\phi \in H^1(\mathbb{R})$ one has for $B > 1$*

$$\begin{aligned}
&\left|\int_{\mathbb{R}} V_{\mathcal{U}}^B(x)\,|\phi(x)|^2\, dx - (\ln B - 2\ln\ln B)\,|\phi(0)|^2\right|\\
&\leq L^{-1}\|\phi\|_2^2 + 8\sqrt{L}\|\phi'\|_2^{3/2}\|\phi\|_2^{1/2}\\
&+ 2\left|\ln L + \ln\ln B + \int_0^\infty e^{-u}\left[\ln\left(\sqrt{1 + \frac{2u}{BL^2}} + 1\right) - \ln\left(\sqrt{2u}\right)\right] du\right| \|\phi'\|_2\|\phi\|_2.
\end{aligned}$$

Proof. Writing

$$\begin{aligned}
\int_{\mathbb{R}} V_{\mathcal{U}}^B(x)|\phi(x)|^2 dx = &\int_{|x|\geq L} V_{\mathcal{U}}^B(x)|\phi(x)|^2 dx\\
&+ \int_{|x|\leq L} V_{\mathcal{U}}^B(x)\left(|\phi(x)|^2 - |\phi(0)|^2\right) dx + |\phi(0)|^2 \int_{|x|\leq L} V_{\mathcal{U}}^B(x) dx
\end{aligned}$$

it is possible to bound

$$\int_{|x|\geq L} V_{\mathcal{U}}^B(x)\,|\phi(x)|^2\, dx \leq \frac{1}{L}\int_{|x|\geq L} |\phi(x)|^2 dx, \tag{3.0.4}$$

$$\left|\int_{|x|\leq L} V_{\mathcal{U}}^B(x)\left(|\phi(x)|^2 - |\phi(0)|^2\right) dx\right| \leq 8\sqrt{L}\|\phi'\|_2^{3/2}\|\phi\|_2^{1/2} \tag{3.0.5}$$

and to evaluate the integral

$$\begin{aligned}\int_{|x|\le L} V_{\mathcal{U}}^{B}(x)\,dx =&2\int_0^\infty e^{-u}\left[\ln\left(\sqrt{L^2+\frac{2u}{B}}+L\right)-\ln\left(\sqrt{\frac{2u}{B}}\right)\right]du\\ &=\ln B+2\ln L+2\int_0^\infty e^{-u}\left[\ln\left(\sqrt{1+\frac{2u}{BL^2}}+1\right)-\ln\sqrt{2u}\right]du.\end{aligned}$$

To arrive at the bound in (3.0.5) the following inequalities are used

$$|\phi(x)-\phi(0)|\le\sqrt{|x|}\|\phi'\|_2 \text{ and } \|\phi\|_\infty\le\|\phi'\|_2^{1/2}\|\phi\|_2^{1/2}. \tag{3.0.6}$$

The bounds from (3.0.4) and (3.0.5) and again using the rightmost inequality of (3.0.6) yield the desired estimate for the lemma.

□

The following corollary is now immediate:

Corollary 9. *For any $L>0$ and $\phi\in H^1(\mathbb{R})$ one has for $B>1$*

$$\begin{aligned}&\left|\int\int_{\mathbb{R}\times\mathbb{R}}|\phi(x)|^2\frac{1}{\sqrt{2}}V_{\mathcal{U}}^{B}\left(\frac{x-y}{\sqrt{2}}\right)|\phi(y)|^2\,dxdy-(\ln B-2\ln\ln B)\|\phi\|_4^4\right|\\ &\le L^{-1}\|\phi\|_2^4+8\sqrt{L}\|\phi'\|_2^{3/2}\|\phi\|_2^{5/2}\\ &+2\left|\ln L+\ln\ln B+\int_0^\infty e^{-u}\left[\ln\left(\sqrt{\frac12+\frac{2u}{BL^2}}+\sqrt{\frac12}\right)-\ln\sqrt{2u}\right]du\right|\|\phi'\|_2\|\phi\|_2^3.\end{aligned}$$

Finally, a link to the one-dimensional minimization problem with a delta-function potential, given in (1.2.6) above, can be established using Lemma 8and Corollary 9. For any $L>0$ and $\phi\in H^1(\mathbb{R})$, $\|\phi\|_{L^2(\mathbb{R})}=1$ one has for $B>1$

$$\begin{aligned}&\mathcal{P}\left(\gamma_B(x_\perp)\,\phi(x_3)\right)\\ &\le B+\int_{\mathbb{R}}|\phi'|\,dx_3-\frac{\alpha}{2}(\ln B-2\ln\ln B)\int_{\mathbb{R}}|\phi|^4\,dx_3-\beta(\ln B-2\ln\ln B)|\phi(0)|^2\\ &+\left(\frac{\alpha}{2}+\beta\right)\left(\frac1L+8\sqrt{L}\|\phi'\|_2^{3/2}+2\|\phi'\|_2\left|\ln(L)+\ln\ln B\right|\right)\\ &+(\alpha+2\beta)\|\phi'\|_2\int_0^\infty e^{-u}\left[\ln\left(\sqrt{1+\frac{2u}{BL^2}}+1\right)+\ln\left(\sqrt{2u}\right)\right]du\end{aligned} \tag{3.0.7}$$

With these observations, we argue the upper bound.

Proof of Theorem 7. We shall denote $\mu(B):=(\ln B-2\ln\ln B)$. Recalling the minimizer $\phi_0$ of the problem given in (1.2.6) for the energy $\mathfrak{e}_0$, we consider

$$f_B(x_3):=\sqrt{\mu(B)}\phi_0((\mu(B))\,x_3).$$

We observe

$$\|f_B\|_2=1,\ \|f_B'\|_2=\mu(B)\,\|\phi_0'\|_2 \tag{3.0.8}$$

and

$$\int_{\mathbb{R}}|f_B'|^2\,dx_3-\alpha\mu(B)\int|f_B|^4\,dx_3-\beta\mu(B)\,|f_B(0)|^2=(\mu(B))^2\,\mathfrak{e}_0. \tag{3.0.9}$$

By the above considerations and choosing $L = (\ln B)^{-1}$ in (3.0.7) above, we deduce using (3.0.8) and (3.0.9) that

$$
\begin{aligned}
&E_0(B) \\
&\leq \inf_{\|\varphi\|_{L^2(\mathbb{R}^3)}=1} \mathcal{P}(\varphi) \\
&\leq \mathcal{P}\left(\gamma_B(x_\perp) f_B(x_3)\right) \\
&= B + \int_{\mathbb{R}} |f_B'|^2 \, dx_3 - \frac{\alpha}{2\sqrt{2}} \int\int_{\mathbb{R}\times\mathbb{R}} |f_B(x_3)|^2 V_{\mathcal{U}}^B \left(\frac{x_3 - y_3}{\sqrt{2}}\right) |f_B(y_3)|^2 \, dx_3 dy_3 \\
&- \beta \int_{\mathbb{R}} |f_B(x_3)|^2 V_{\mathcal{U}}^B (x_3) \, dx_3 \\
&\leq B + \int_{\mathbb{R}} |f_B'|^2 \, dx_3 - \frac{\alpha}{2} \mu(B) \int_{\mathbb{R}} |f_B(x_3)|^4 \, dx_3 - \beta \mu(B) |f_B(0)|^2 \\
&+ \left(\frac{\alpha}{2} + \beta\right) \left(\ln B + 8 (\ln B)^{-1/2} \|f_B'\|_2^{3/2}\right) \\
&+ (\alpha + 2\beta) \|f_B'\|_2 \int_0^\infty e^{-u} \left[\ln\left(\sqrt{1 + \frac{2u (\ln B)^2}{B}} + 1\right) + \ln\left(\sqrt{2u}\right)\right] du \\
&= B + \mathfrak{e}_0 (\mu(B))^2 + \left(\frac{\alpha}{2} + \beta\right) \Bigg(\ln B + \frac{8 (\mu(B))^{3/2}}{(\ln B)^{1/2}} \|\phi_0'\|_2^{3/2} \\
&+ 2\mu(B) \|\phi_0'\|_2 \int_0^\infty e^{-u} \left[\ln\left(\sqrt{1 + \frac{2u (\ln B)^2}{B}} + 1\right) + \ln\left(\sqrt{2u}\right)\right] du\Bigg) \\
&\leq B + \mathfrak{e}_0 \left((\ln B)^2 - 4 (\ln B)(\ln \ln B)\right) + C (\ln B)
\end{aligned}
$$

The desired estimate now follows.

□

Corollary 10. *For $W$ a sum of a bounded Borel measure on the real line and a $L^\infty(\mathbb{R})$-function, $E_\epsilon(B)$ the ground-state energy of the perturbed Hamiltonian in (1.2.10) and $\mathfrak{e}_\epsilon$ as given in (1.2.12) there is a constant $C > 0$ such that for $B > 1$*

$$E_\epsilon(B) \leq B + \mathfrak{e}_\epsilon (\ln B)^2 + C \ln B \ln \ln B.$$

Proof. From (2.0.14) $\mathfrak{e}_\epsilon > -\infty$, and for $B > 1$ there exists some $\phi_B \in H^1(\mathbb{R})$, $\|\phi_B\|_2 = 1$ satisfying

$$
\begin{aligned}
&\int_{\mathbb{R}} |\phi_B'|^2 \, dx_3 - \frac{\alpha}{2} \int_{\mathbb{R}} |\phi_B(x_3)|^4 \, dx_3 - \beta |\phi_B(0)|^2 - \epsilon \int_{\mathbb{R}} W(x_3) |\phi_B(x_3)|^2 \, dx_3 \\
&< \mathfrak{e}_\epsilon + (\ln B)^{-1}.
\end{aligned} \tag{3.0.10}
$$

Denoting $g_B(x_3) := \sqrt{\ln B}\phi_B((\ln B) x_3)$ we observe $\|g_B\|_2 = 1$, $\|g_B'\|_2 = (\ln B) \|\phi_B'\|_2$ and, by (3.0.10),

$$
\begin{aligned}
&\int_{\mathbb{R}} |g_B'|^2 \, dx_3 - \frac{\alpha}{2} \int_{\mathbb{R}} |g_B(x_3)|^4 \, dx_3 - \beta |g_B(0)|^2 - \epsilon \int_{\mathbb{R}} W(x_3) |g_B(x_3)|^2 \, dx_3 \\
&\leq (\ln B)^2 \mathfrak{e}_\epsilon + (\ln B).
\end{aligned}
$$

As above,

$$
\begin{aligned}
&E_\epsilon(B) \\
&\leq \inf_{\|\varphi\|_{L^2(\mathbb{R}^3)}=1} \left( \mathcal{P}(\varphi) - \epsilon (\ln B)^2 \int_{\mathbb{R}} W((\ln B) x_3) \left( \int_{\mathbb{R}^2} |\varphi(x_\perp, x_3)|^2 \, dx_\perp \right) dx_3 \right) \\
&\leq \mathcal{P}(\gamma_B(x_\perp) g_B(x_3)) - \epsilon (\ln B)^2 \int_{\mathbb{R}} W((\ln B) x_3) |g_B(x_3)|^2 \, dx_3 \\
&\leq B + \int_{\mathbb{R}} |g_B'|^2 \, dx_3 - \frac{\alpha \ln B}{2} \int_{\mathbb{R}} |g_B(x_3)|^4 \, dx_3 - \beta (\ln B) |g_B(0)|^2 \\
&\quad - \epsilon (\ln B)^2 \int_{\mathbb{R}} W((\ln B) x_3) |g_B(x_3)|^2 \, dx_3 \\
&\quad + \left( \frac{\alpha}{2} + \beta \right) \left( L^{-1} + 8\sqrt{L} \|g_B'\|_2^{3/2} + 2\|g_B'\|_2 |\ln(L)| \right) \\
&\quad + (\alpha + 2\beta) \|g_B'\|_2 \int_0^\infty e^{-u} \left[ \ln \left( \sqrt{1 + \frac{2u}{BL^2}} + 1 \right) + \ln \left( \sqrt{2u} \right) \right] du \\
&\leq B + \mathfrak{e}_\epsilon \ln B + \ln B \\
&\quad + \left( \frac{\alpha}{2} + \beta \right) \left( L^{-1} + 8\sqrt{L} (\ln B)^{3/2} \|\phi_B'\|_2^{3/2} + 2 (\ln B) \|\phi_B'\|_2 |\ln(L)| \right) \\
&\quad + (\alpha + 2\beta)(\ln B) \|\phi_B'\|_2 \int_0^\infty e^{-u} \left[ \ln \left( \sqrt{1 + \frac{2u}{BL^2}} + 1 \right) + \ln \left( \sqrt{2u} \right) \right] du
\end{aligned}
$$

Since, by (3.0.10) and the estimate in (2.0.14) above, $\|\phi_B'\|_2 < C$ for all $B > 1$, the desired estimate now follows from choosing $L = (\ln B)^{-1}$.

$\square$

CHAPTER 4

# Lower Bound for the Ground-State Energy and Main Result

The goal of this chapter is to prove the following theorem:

THEOREM 11. *There is a constant $C > 0$ such that for all $B \geq C$*

$$E_0(B) \geq B - \mathfrak{e}_0 (\ln B)^2 - C (\ln B)^{3/2}.$$

The proof of Theorem 11 shall be given at the end of Subsection 4.2. The arguments will follow [FG2015] with some modifications. The essential idea is to show that in a strong magnetic field the ground state is concentrated in the lowest Landau level. It is then possible to extract a one-dimensional Hamiltonian to which the Lieb-Thomas argument is applied to extract as a lower bound the one-dimensional functional yielding the desired second leading-order term of the ground-state energy.

Theorem 1 follows from Theorem 11 and Theorem 7.

In this Chapter $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$ shall be used to denote the norm and inner product on $L^2(\mathbb{R}^3) \otimes \mathcal{F}$. For $\Psi \in H^1_A(\mathbb{R}^3) \otimes \mathcal{F}$ its electron density in the direction of the magnetic field shall be denoted $\tilde{\Psi}^2(x_3)$ i.e.

$$\tilde{\Psi}(x_3) := \left( \int_{\mathbb{R}^2} \|\Psi\|^2_{\mathcal{F}} (x_\perp, x_3)\, dx_\perp \right)^{\frac{1}{2}}.$$

By Hölder's inequality $\|\partial_3 \tilde{\Psi}\|_2 \leq \|\partial_3 \Psi\|$ and $\tilde{\Psi} \in H^1(\mathbb{R})$. Furthermore the integral operator $P_0^B$ acting on $L^2(\mathbb{R}^2)$ with kernel

$$P_0^B(x_\perp, y_\perp) = \frac{B}{2\pi} e^{-\frac{B}{4}|x_\perp - y_\perp|^2} e^{\frac{iB}{2}(x_1 y_2 - x_2 y_1)} \tag{4.0.1}$$

is the projection onto the lowest Landau level i.e. the ground state of the two-dimensional Landau Hamiltonian $H_B$. The operators $P_0^B \otimes 1$ and $P_0^B \otimes 1 \otimes 1$ acting respectively on $L^2(\mathbb{R}^2) \otimes L^2(\mathbb{R})$ and $L^2(\mathbb{R}^2) \otimes L^2(\mathbb{R}) \otimes \mathcal{F}$ shall also be denoted $P_0^B$.

## 4.1. Bathtub Principle

The results in this section will be useful later for extracting the delta-function potential as a lower bound from the Coulomb potential after projecting onto the lowest Landau level.

LEMMA 12. *For any $L > 0$ and $\Psi \in H^1_A(\mathbb{R}^3) \otimes \mathcal{F}$ one has for $B > 1$*

$$\int_{\mathbb{R}^3} \frac{\left\|P_0^B \Psi\right\|^2_{\mathcal{F}} (x_\perp, x_3)}{\sqrt{|x_\perp|^2 + x_3^2}}\, dx_\perp dx_3 - (\ln B - 2 \ln\ln B) \left(\tilde{\Psi}(0)\right)^2$$
$$\leq L^{-1} \|\tilde{\Psi}\|_2^2 + 8\sqrt{L} \|\partial_3 \tilde{\Psi}\|_2^{3/2} \|\tilde{\Psi}\|_2^{1/2} + |\mathcal{D}(B, L)|\, \|\partial_3 \tilde{\Psi}\|_2 \|\tilde{\Psi}\|_2,$$

*where*

$$\mathcal{D}\left(B,L\right):=2\ln L+2\ln\ln B+\frac{2}{\sqrt{\frac{2}{BL^2}+1}+1}+2\ln\left(\sqrt{1+\frac{2}{BL^2}}+1\right)-\ln 2. \tag{4.1.1}$$

Proof. By Hölder's inequality

$$\left\|P_0^B\Psi\right\|_{\mathcal{F}}^2\left(x_\perp,x_3\right)\leq\left(\frac{B}{2\pi}\right)\left(\tilde{\Psi}\left(x_3\right)\right)^2, \tag{4.1.2}$$

and since $P_0^B$ is a projection

$$\int_{\mathbb{R}^3}\left\|P_0^B\Psi\right\|_{\mathcal{F}}^2\left(x_\perp,x_3\right)dx_\perp dx_3\leq\int_{\mathbb{R}}\left(\tilde{\Psi}\left(x_3\right)\right)^2dx_3. \tag{4.1.3}$$

It follows from the Bathtub principle [**LL2001**] that the maximum of the expression

$$\int_{\mathbb{R}^2}\frac{G\left(x_\perp,x_3\right)}{\sqrt{\left|x_\perp\right|^2+x_3}}dx_\perp$$

over all functions $G$ satisfying the conditions (4.1.2) and (4.1.3) above is attained by the function

$$G_{\max}\left(x_\perp,x_3\right)=\begin{cases}\left(\frac{B}{2\pi}\right)\left(\tilde{\Psi}\left(x_3\right)\right)^2 & \text{when}\quad\left|x_\perp\right|\leq R\\ 0 & \text{when}\quad\left|x_\perp\right|>R\end{cases}$$

where $R=\sqrt{\frac{2}{B}}$. Therefore

$$\begin{aligned}\int_{\mathbb{R}}\int_{\mathbb{R}^2}\frac{\left\|P_0^B\Psi\right\|_{\mathcal{F}}^2\left(x_\perp,x_3\right)}{\sqrt{\left|x_\perp\right|^2+x_3^2}}dx_\perp dx_3&\leq\int_{\mathbb{R}}\int_{\left|x_\perp\right|\leq\sqrt{\frac{2}{B}}}\frac{G_{\max}\left(x_\perp,x_3\right)}{\sqrt{\left|x_\perp\right|^2+x_3^2}}dx_\perp dx_3\\&=\int_{\mathbb{R}}V_{\mathcal{L}}^B(x_3)\left(\tilde{\Psi}\left(x_3\right)\right)^2dx_3\end{aligned}$$

with the effective Coulomb potential

$$V_{\mathcal{L}}^B(x_3):=\frac{2}{\sqrt{\frac{2}{B}+x_3^2}+|x_3|}. \tag{4.1.4}$$

Now the theorem follows from Lemma 13 given below.

∎

Lemma 13. *For any $L>0$ and $\phi\in H^1(\mathbb{R})$ one has for B>1*

$$\begin{aligned}&\int_{\mathbb{R}}V_{\mathcal{L}}^B(x)\left|\phi\left(x\right)\right|^2dx-\left(\ln B-2\ln\ln B\right)\left|\phi\left(0\right)\right|^2\\&\leq L^{-1}\|\phi\|_2^2+8\sqrt{L}\|\phi'\|_2^{3/2}\|\phi\|_2^{1/2}+|\mathcal{D}(B,L)|\,\|\phi'\|_2\|\phi\|_2,\end{aligned}$$

*where*

$$\mathcal{D}\left(B,L\right):=2\ln L+2\ln\ln B+\frac{2}{\sqrt{\frac{2}{BL^2}+1}+1}+2\ln\left(\sqrt{1+\frac{2}{BL^2}}+1\right)-\ln 2.$$

PROOF. The lemma follows as in the proof of Lemma 8 and from evaluating the integral

$$\int_{|x|<L} V_{\mathcal{L}}^{B}(x)\, dx = \ln B - 2\ln\ln B + \mathcal{D}\left(B, L\right).$$

$\square$

COROLLARY 14. *Let $\tau > 0$. There is a constant $C > 0$ such that for all $B \geq C$ and $\Psi \in H_A^1\left(\mathbb{R}^3\right) \otimes \mathcal{F}$*

$$\|\partial_3 \Psi\|^2 - \tau \left\langle \Psi,\, P_0^B\, |x|^{-1}\, P_0^B \Psi \right\rangle \geq \left( -\frac{\tau^2}{4} \left(\ln B\right)^2 + \tau^2 \ln B \ln\ln B - C\left(\ln B\right) \right) \|\Psi\|^2$$

PROOF. Recall for $\epsilon > 0$, $\|\partial_3 \tilde{\Psi}\|_2 \|\tilde{\Psi}\|_2 \leq \epsilon \|\partial_3 \tilde{\Psi}\|_2^2 + \epsilon^{-1}\|\tilde{\Psi}\|_2^2$. With $\mathcal{D}\left(B, L\right)$ as given in (4.1.1), under the assumption that $2\tau\epsilon\left|\mathcal{D}\left(B, L\right)\right| < 1/2$ and denoting $\mu(B) := \left(\ln B - 2\ln\ln B\right)$ it follows from Lemma 12 that

$$\begin{aligned}
&\|\partial_3 \Psi\|^2 - \tau \left\langle \Psi,\, P_0^B\, |x|^{-1}\, P_0^B \Psi \right\rangle \\
&\geq \left(1 - 2\tau\epsilon\left|\mathcal{D}\left(B, L\right)\right|\right) \|\partial_3 \tilde{\Psi}\|_2^2 - \tau \mu(B) \left(\tilde{\Psi}(0)\right)^2 - \tau\left(L^{-1} + \epsilon^{-1}\left|\mathcal{D}\left(B, L\right)\right|\right) \|\tilde{\Psi}\|_2^2 \\
&\quad + \tau\epsilon\left|\mathcal{D}\left(B, L\right)\right| \|\partial_3 \tilde{\Psi}\|_2^2 - 8\tau\sqrt{L}\|\tilde{\Psi}\|_2^{1/2}\|\partial_3\tilde{\Psi}\|_2^{3/2} \\
&\geq -\frac{\tau^2\left(\mu(B)\right)^2}{4\left(1 - 2\tau\epsilon\left|\mathcal{D}\left(B, L\right)\right|\right)}\|\tilde{\Psi}\|_2^2 - \tau\left(\frac{432 L^2}{\left|\mathcal{D}\left(B, L\right)\right|^3 \epsilon^3} + L^{-1} + \epsilon^{-1}\left|\mathcal{D}\left(B, L\right)\right|\right)\|\tilde{\Psi}\|_2^2 \\
&\geq \left(\left(-\frac{\tau^2}{4} - \tau^3\epsilon\left|\mathcal{D}\left(B, L\right)\right|\right)\left(\mu(B)\right)^2 - \frac{432\tau L^2}{\left|\mathcal{D}\left(B, L\right)\right|^3\epsilon^3} - \frac{\tau}{L} - \frac{\tau\left|\mathcal{D}\left(B, L\right)\right|}{\epsilon}\right)\|\tilde{\Psi}\|_2^2.
\end{aligned}$$

At the second inequality it is used that $\|\partial_3\tilde{\Psi}\|_2^2 - \zeta(\tilde{\Psi}(0))^2 \geq -(1/4)\zeta^2\|\tilde{\Psi}\|_2^2$ for $\zeta \geq 0$ and that $ax^2 - bx^{3/2} \geq -(27/256)b^4/a^3$ for $a > 0, b \geq 0$ and $x \geq 0$. Now choosing $\epsilon = \left(\ln B\right)^{-1}$ and $L = \left(\ln B\right)^{-1}$ the above assumption, $2\tau\epsilon\left|\mathcal{D}\left(B, L\right)\right| < 1/2$, can be verified to be true for all $B \geq C$. The lemma follows.

$\square$

## 4.2. Lowest Landau Level

The goal of this section is to argue that for large $B$ the ground state is concentrated in the lowest Landau level.

For $\mathcal{K} > 0$ define the cut-off Hamiltonian

$$\begin{aligned}
\mathfrak{h}_{\mathcal{K}}^{\mathrm{co}} := \left(1 - \frac{8\alpha}{\pi\mathcal{K}}\right)\left(H_B - \partial_3^2\right) + \frac{1}{2}\int_{\Gamma_{\mathcal{K}}} a_k^\dagger a_k\, dk + \frac{1}{2}\mathcal{N} \\
+ \frac{\sqrt{\alpha}}{2\pi}\int_{\Gamma_{\mathcal{K}}}\left(\frac{a_k e^{ik\cdot x}}{|k|} + \frac{a_k^\dagger e^{-ik\cdot x}}{|k|}\right) dk
\end{aligned}$$

with $\Gamma_{\mathcal{K}} = \{k \in \mathbb{R}^3 : \max\left(|k_\perp|, |k_3|\right) \leq \mathcal{K}\}$.

LEMMA 15. *For $\mathcal{K} > \frac{8\alpha}{\pi}$*

$$\mathbb{H}(B) \geq \mathfrak{h}_{\mathcal{K}}^{co} - \beta\,|x|^{-1} - 1/4.$$

PROOF. See Lemma 5.1 in [**FG2015**].

$\square$

Lemma 16. *There exists a constant $C > 0$ such that for all $B \geq C$*

$$\mathbb{H}(B) \geq \left(1 - \frac{8\alpha \left(\ln B\right)^2}{\pi B}\right) H_B + \left(\frac{1}{2} - \frac{8\alpha \left(\ln B\right)^2}{\pi B}\right) \left(-\partial_3^2\right) - \beta \left|x\right|^{-1} + \frac{1}{2}\mathcal{N} - C \left(\ln B\right)^2 .$$

Proof. Let $\mathcal{K} = B/\left(\ln B\right)^2$ and $\mathcal{K}_3 = 16\alpha \left|\ln B\right|/\pi$. By completion of square

$$\begin{aligned}
\int_{|k_3|\leq \mathcal{K}_3} \int_{|k_\perp|\leq \mathcal{K}} &\left(\frac{1}{2}a_k^\dagger a_k + \frac{\sqrt{\alpha}}{2\pi}\frac{a_k}{|k|}e^{ik\cdot x} + \frac{\sqrt{\alpha}}{2\pi}\frac{a_k^\dagger}{|k|}e^{-ik\cdot x}\right) dk_\perp dk_3 \\
&\geq -\frac{\alpha}{2\pi^2}\int_{|k_3|\leq \mathcal{K}_3}\int_{|k_\perp|\leq \mathcal{K}} \frac{1}{|k|^2} dk_\perp dk_3 \\
&= -\frac{\alpha}{\pi}\int_0^{\mathcal{K}_3} \ln\left(\frac{\mathcal{K}^2 + \mathcal{K}_3^2}{\mathcal{K}_3^2}\right) dk_3 \\
&= -\frac{\alpha}{\pi}\left(\mathcal{K}_3 \ln\left(\frac{\mathcal{K}^2}{\mathcal{K}_3^2} + 1\right) + 2\mathcal{K}\arctan\left(\frac{\mathcal{K}_3}{\mathcal{K}}\right)\right) \\
&\geq -\frac{\alpha}{\pi}\mathcal{K}_3\left(\ln\left(\frac{\mathcal{K}^2}{\mathcal{K}_3^2} + 1\right) + 2 + \frac{2}{3}\frac{\mathcal{K}_3^2}{\mathcal{K}^2}\right) \\
&\geq -C\left(\ln B\right)^2 , \qquad (4.2.1)
\end{aligned}$$

valid for some constant $C$ and all $B \geq C$.

Denoting $\Lambda\left(B\right) = \{(k_\perp, k_3) \in \Gamma_{\mathcal{K}} : \mathcal{K}_3 \leq |k_3| \leq \mathcal{K} \text{ and } |k_\perp| \leq \mathcal{K}\}$ it can be argued as in the proof of Lemma 5.2 in [**FG2015**] that for $B$ large

$$\frac{\sqrt{\alpha}}{2\pi}\int_{\Lambda(B)}\left(\frac{a_k}{|k|}e^{ik\cdot x} + \frac{a_k^\dagger}{|k|}e^{-ik\cdot x}\right) dk \geq \frac{1}{2}\partial_3^2 - \frac{1}{2}\left(\int_{\Lambda(B)} a_k^\dagger a_k dk + \frac{1}{2}\right). \qquad (4.2.2)$$

The lemma now follows from Lemma 15, the estimates (4.2.1) and (4.2.2) and the non-negativity of $\mathcal{N}$.

□

Lemma 17. *There exists a constant $C > 0$ such that for all $B \geq C$ and all $\Psi \in H_A^1\left(\mathbb{R}^3\right)\otimes$ dom$\left(\sqrt{\mathcal{N}}\right)$ with $\|\Psi\| = 1$*

$$\langle \Psi, \mathbb{H}(B)\Psi\rangle \geq B + \frac{B}{2}\|P_>^B\Psi\|^2 + \frac{1}{2}\left\langle \Psi, \mathcal{N}\Psi\right\rangle - C\left(\ln B\right)^2 .$$

Proof. Below $0 < \eta < 1$ and $\mathcal{A} > 1$. By the diamagnetic inequality

$$\left\langle \Psi, \left(H_B - \partial_3^2\right)\Psi\right\rangle \geq \mathcal{A}\left\langle \Psi,\, \beta|x|^{-1}\Psi\right\rangle - 4^{-1}\beta^2\mathcal{A}^2\|\Psi\|^2.$$

Then writing $\theta = \left(\frac{1}{2} - \frac{8\alpha(\ln B)^2}{\pi B}\right)$ for $B$ large

$$\begin{aligned}
&\theta\left\langle \Psi, \left(H_B - \partial_3^2\right)\Psi\right\rangle - \left\langle \Psi,\, \beta|x|^{-1}\Psi\right\rangle \\
&= \theta\left\langle P_0^B\Psi, \left(H_B - \partial_3^2\right)P_0^B\Psi\right\rangle - \left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle \\
&\quad + \theta\left(1-\eta\right)\left\langle P_>^B\Psi, \left(H_B - \partial_3^2\right)P_>^B\Psi\right\rangle + \theta\eta\left\langle P_>^B\Psi, \left(H_B - \partial_3^2\right)P_>^B\Psi\right\rangle \\
&\quad - \left\langle P_>^B\Psi,\, \beta|x|^{-1}P_>^B\Psi\right\rangle - \left\langle P_0^B\Psi,\, \beta|x|^{-1}P_>^B\Psi\right\rangle - \left\langle P_>^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle
\end{aligned}$$

$$\geq \theta \left\langle P_0^B\Psi, \left(H_B - \partial_3^2\right) P_0^B\Psi\right\rangle - \left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle$$
$$+ \theta\left(1-\eta\right)\left\langle P_>^B\Psi, \left(H_B - \partial_3^2\right) P_>^B\Psi\right\rangle - \mathcal{A}^2\beta^2\left(4\theta\eta\right)^{-1}\left\|P_>^B\Psi\right\|^2$$
$$+ \left(\mathcal{A}-1\right)\left\langle P_>^B\Psi,\, \beta|x|^{-1}P_>^B\Psi\right\rangle - 2\left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle^{\frac{1}{2}}\left\langle P_>^B\Psi,\, \beta|x|^{-1}P_>^B\Psi\right\rangle^{\frac{1}{2}}$$

$$\geq \theta\left\langle P_0^B\Psi, H_B P_0^B\Psi\right\rangle + \left[\theta\left\langle P_0^B\Psi, -\partial_3^2 P_0^B\Psi\right\rangle - \left(\mathcal{A}/(\mathcal{A}-1)\right)\left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle\right]$$
$$+ \theta\left(1-\eta\right)\left\langle P_>^B\Psi, \left(H_B - \partial_3^2\right) P_>^B\Psi\right\rangle - \mathcal{A}^2\beta^2\left(4\theta\eta\right)^{-1}\left\|P_>^B\Psi\right\|^2$$

$$\geq \theta B + \left[\theta\left\langle P_0^B\Psi, -\partial_3^2 P_0^B\Psi\right\rangle - \left(\mathcal{A}/(\mathcal{A}-1)\right)\left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle\right]$$
$$+ \left(3\theta B/2\right)\left\|P_>^B\Psi\right\|^2 + \left[\theta\left(B/2 - 3B\eta\right) - \mathcal{A}^2\beta^2\left(4\theta\eta\right)^{-1}\right]\left\|P_>^B\Psi\right\|^2.$$

Choose $\eta = 1/12$ and $\mathcal{A} = \theta\beta^{-1}\left(B/48\right)^{\frac{1}{2}}$. For $B$ large $\left(\mathcal{A}/(\mathcal{A}-1)\right) < 2$ and by Corollary 14 there exists some $C > 0$ such that for all $B \geq C$

$$\theta\left\langle P_0^B\Psi, -\partial_3^2 P_0^B\Psi\right\rangle - \left(\mathcal{A}/(\mathcal{A}-1)\right)\left\langle P_0^B\Psi,\, \beta|x|^{-1}P_0^B\Psi\right\rangle \geq -C\left(\ln B\right)^2.$$

The lemma now follows from Lemma 16. $\square$

The following observation is immediate from Theorem 7: For every $M > \mathfrak{e}_0$ there are states $\Psi \in H_A^1(\mathbb{R}^3) \otimes \operatorname{dom}\left(\sqrt{\mathcal{N}}\right)$ satisfying

$$\left\langle \Psi, \mathbb{H}(B)\Psi\right\rangle \leq B + M\left(\ln B\right)^2 \quad \text{and} \quad \|\Psi\| = 1. \tag{4.2.3}$$

Corollary 18. *For every $M \in \mathbb{R}$ there is a constant $C_M > 0$ such that for every $B \geq C_M$ and every $\Psi \in H_A^1(\mathbb{R}^3) \otimes$ dom$\left(\sqrt{\mathcal{N}}\right)$ satisfying* (4.2.3)

$$\|P_>^B\Psi\|^2 \leq C_M\left(\ln B\right)^2 B^{-1} \quad \text{and} \quad \left\langle \Psi, \mathcal{N}\Psi\right\rangle \leq C_M\left(\ln B\right)^2.$$

Proof. The corollary follows from (4.2.3) and Lemma 17. $\square$

Lemma 19. *Let $\mathcal{K} > 8\alpha/\pi$ and $1 < \mathcal{A} < \left(B/\ln B\right)^{1/2}$. Denoting $\kappa = \left(1 - (8\alpha/\pi\mathcal{K})\right)$ for every $M \in \mathbb{R}$ there is a $C_M > 0$ such that for all $B \geq C_M$ and $\Psi \in H_A^1(\mathbb{R}^3) \otimes$ dom$\left(\sqrt{\mathcal{N}}\right)$ satisfying (4.2.3)*

$$\left\langle \Psi, \mathbb{H}(B)\Psi\right\rangle \geq \left\langle P_0^B\Psi, \left(\mathfrak{h}_{\mathcal{K}}^{co} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)|x|^{-1}\right)P_0^B\Psi\right\rangle + \kappa B\|P_>^B\Psi\|^2$$
$$- C_M\left(\ln B\right)^2\left(\mathcal{K}B^{-1} + \sqrt{\mathcal{K}B^{-1}}\right) - C_M\kappa^{-1}\ln B - 1/4.$$

Proof. It can be argued as in the proof of Lemma 17 with $0 < \eta < 1$

$$\kappa\left\langle \Psi, \left(H_B - \partial_3^2\right)\Psi\right\rangle - \left\langle \Psi,\, \beta|x|^{-1}\Psi\right\rangle$$
$$\geq \kappa\left\langle P_0^B\Psi, \left(H_B - \partial_3^2\right)P_0^B\Psi\right\rangle - \left(\mathcal{A}/\left(\mathcal{A}-1\right)\right)\left\langle P_0^B\Psi, \beta|x|^{-1}P_0^B\Psi\right\rangle$$
$$+ \kappa B\left\|P_>^B\Psi\right\|^2 + \left[\kappa\left(2B - 3B\eta\right) - \mathcal{A}^2\beta^2\left(4\eta\kappa\right)^{-1}\right]\left\|P_>^B\Psi\right\|^2.$$

It now follows from Lemma 15 that

$$\begin{aligned}\langle\Psi,\mathbb{H}(B)\Psi\rangle \geq &\left\langle P_0^B\Psi, \left(\mathfrak{h}_{\mathcal{K}}^{\rm co}-\beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)|x|^{-1}\right)P_0^B\Psi\right\rangle+\kappa B\|P_>^B\Psi\|^2\\ &+\left[\kappa\left(2B-3B\eta\right)-\mathcal{A}^2\beta^2\left(4\eta\kappa\right)^{-1}\right]\left\|P_>^B\Psi\right\|^2-\frac{1}{4}\\ &+\left\langle P_>^B\Psi,\ \left(\int_{\Gamma_{\mathcal{K}}}a_k^\dagger a_k+\frac{\sqrt{\alpha}}{2\pi}\frac{a_ke^{ik\cdot x}}{|k|}+\frac{\sqrt{\alpha}}{2\pi}\frac{a_k^\dagger e^{-ik\cdot x}}{|k|}dk\right)P_>^B\Psi\right\rangle\\ &+\left\langle P_0^B\Psi,\ \left(\frac{\sqrt{\alpha}}{2\pi}\int_{\Gamma_{\mathcal{K}}}\frac{a_ke^{ik\cdot x}}{|k|}+\frac{a_k^\dagger e^{-ik\cdot x}}{|k|}dk\right)P_>^B\Psi\right\rangle\\ &+\left\langle P_>^B\Psi,\ \left(\frac{\sqrt{\alpha}}{2\pi}\int_{\Gamma_{\mathcal{K}}}\frac{a_ke^{ik\cdot x}}{|k|}+\frac{a_k^\dagger e^{-ik\cdot x}}{|k|}dk\right)P_0^B\Psi\right\rangle.\end{aligned}$$

By completion of square

$$\begin{aligned}&\int_{\Gamma_{\mathcal{K}}}\left(a_k^\dagger a_k+\frac{\sqrt{\alpha}}{2\pi}\frac{a_k}{|k|}e^{ik\cdot x}+\frac{\sqrt{\alpha}}{2\pi}\frac{a_k^\dagger}{|k|}e^{-ik\cdot x}\right)dk\\ &\geq -\frac{\alpha}{4\pi^2}\int_{\Gamma_{\mathcal{K}}}\frac{1}{|k|^2}\,dk_\perp dk_3\\ &=-\frac{\alpha\left(2\ln(2)+\pi\right)}{4\pi}\mathcal{K},\end{aligned}$$

and by Corollary 18 for $B\geq C_M$

$$\begin{aligned}&\left\langle P_>^B\Psi,\ \left(\int_{\Gamma_{\mathcal{K}}}a_k^\dagger a_k+\frac{\sqrt{\alpha}}{2\pi}\frac{a_ke^{ik\cdot x}}{|k|}+\frac{\sqrt{\alpha}}{2\pi}\frac{a_k^\dagger e^{-ik\cdot x}}{|k|}dk\right)P_>^B\Psi\right\rangle\\ &\geq -\frac{\alpha\left(2\ln(2)+\pi\right)}{4\pi}\mathcal{K}\|P_>^B\Psi\|^2\\ &\geq -C_M\mathcal{K}B^{-1}\left(\ln B\right)^2.\end{aligned}$$

Furthermore it can be argued as in the proof of Lemma 5.4 in [**FG2015**] and using Corollary 18 that for $B\geq C_M$

$$\begin{aligned}&\left|\left\langle P_0^B\Psi,\ \left(\frac{\sqrt{\alpha}}{2\pi}\int_{\Gamma_{\mathcal{K}}}\frac{a_k}{|k|}e^{ik\cdot x}dk\right)P_>^B\Psi\right\rangle\right|\\ &\leq C\sqrt{\mathcal{K}}\|P_>^B\Psi\|\|\sqrt{\mathcal{N}+1}P_0^B\Psi\|\\ &\leq C_M\sqrt{\mathcal{K}B^{-1}}\left(\ln B\right)^2.\end{aligned}$$

The remaining interaction terms are estimated similarly. Choosing $\eta=2/3$ the lemma follows from Corollary 18.

$\square$

PROPOSITION 20. *There is a constant $C>0$ such that for all $B,\kappa,\mathcal{K}$ and $\mathcal{A}$ satisfying $B\geq C$, $C\left(\ln B\right)^{-1/2}\leq\kappa\leq C^{-1}\ln B$, $\mathcal{K}\geq\sqrt{B}$ and $1<\mathcal{A}<\left(B/\ln B\right)^{1/2}$*

$$\begin{aligned}&\left\langle P_0^B\Psi,\left(\mathfrak{h}_{\mathcal{K}}^{co}-\beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)|x|^{-1}\right)P_0^B\Psi\right\rangle\\ &\geq\left(\kappa B+\kappa^{-1}\left(\ln B\right)^2\mathfrak{e}_0-C\kappa^{-1/2}\left(\ln B\right)^{3/2}-C\left(1+\kappa^{-1}\right)\ln B\right)P_0^B\end{aligned}$$

A proof of Proposition 20 shall be provided in Subsection 4.3.

Proof of Theorem 11. Fix $M > \mathfrak{e}_0$. By Theorem 7 there are wave functions satisfying (4.2.3). It suffices to argue the desired lower bound on $\langle \Psi, \mathbb{H}(B)\Psi\rangle$ with those wave functions. By Theorem 19 and Proposition 20

$$\begin{aligned}
&\langle \Psi, \mathbb{H}(B)\Psi\rangle \\
&\geq \kappa B + \left(\kappa^{-1}(\ln B)^2 \mathfrak{e}_0 - C\kappa^{-1/2}(\ln B)^{3/2} - C\left(1+\kappa^{-1}\right)\ln B\right)\left\|P_0^B\Psi\right\|^2 \\
&\quad - C(\ln B)^2\left(\mathcal{K}B^{-1} + \sqrt{\mathcal{K}B^{-1}}\right) - C\kappa^{-1}\ln B - C
\end{aligned}$$

with $\kappa = (1-(8\alpha/\pi\mathcal{K}))$. Choosing $\mathcal{K} = B(\ln B)^{-4/3}$ and since $\left\|P_0^B\Psi\right\| \leq 1$

$$\langle \Psi, \mathbb{H}(B)\Psi\rangle \geq B + \mathfrak{e}_0(\ln B)^2 - C(\ln B)^{3/2},$$

which is the claimed lower bound.

□

### 4.3. Proof of Proposition 20.

The proof will proceed in several steps. First there will be a reduction to an essentially one-dimensional Hamiltonian to which a one-dimensional Lieb-Thomas argument is applied to extract the one-dimensional functional as a lower bound.

**Reduction to "one dimension"**. In [**FG2015**] the authors consider a "one-dimensional" Hamiltonian with $0 < \mathcal{K}_3 \leq \mathcal{K}$ and $1 \leq \mathcal{K}_\perp \leq \mathcal{K}$

$$\begin{aligned}
&\mathfrak{h}^{1\mathrm{d}} := \\
&\kappa_1\left(-\partial_3^2\right) + \int_{|k_3|\leq \mathcal{K}_3} \widehat{a}_{k_3}^\dagger \widehat{a}_{k_3} dk_3 + \frac{\sqrt{\alpha}}{2\pi}\int_{|k_3|\leq\mathcal{K}_3} \nu(k_3)\left(\widehat{a}_{k_3}e^{ik_3x_3} + \widehat{a}_{k_3}^\dagger e^{-ik_3x_3}\right)dk_3
\end{aligned}$$

acting on $L^2(\mathbb{R}^3)\otimes\mathcal{F}$ with

$$\kappa_1 := \kappa - \frac{8\alpha}{\pi\mathcal{K}_3}\int_0^\infty e^{-\frac{\mathcal{K}_3^2 t}{2B}}\frac{1}{1+t}\,dt$$

and $\kappa$ as in the statement of Proposition 20, and

$$\widehat{a}_{k_3} := \frac{1}{\nu(k_3)}\int_{1\leq|k_\perp|\leq\mathcal{K}_\perp}\frac{a_k}{|k|}e^{ik_\perp\cdot x_\perp}dk_\perp$$

with

$$\nu(k_3) := \left(\int_{1\leq|k_\perp|\leq\mathcal{K}_\perp}|k|^{-2}\,dk_\perp\right)^{\frac{1}{2}} = \sqrt{\pi}\left(\ln\left(\mathcal{K}_\perp^2 + k_3^2\right) - \ln\left(1+k_3^2\right)\right)^{\frac{1}{2}}.$$

Furthermore $[\widehat{a}_{k_3}, \widehat{a}_{k_3'}^\dagger] = \delta(k_3 - k_3')$ and $\left[\widehat{a}_{k_3}, \widehat{a}_{k_3'}\right] = [\widehat{a}_{k_3}^\dagger, \widehat{a}_{k_3'}^\dagger] = 0$ for $k_3, k_3' \in \mathbb{R}$.

Lemma 21. *Denoting* $\kappa_2 = \kappa - 2\alpha\pi^{-1}\mathcal{K}_3\mathcal{K}_\perp^{-1}$

$$\begin{aligned}
&P_0^B\left(\mathfrak{h}_{\mathcal{K}}^{co} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)|x|^{-1}\right)P_0^B \\
&\geq \kappa_2 B P_0^B + P_0^B\left(\mathfrak{h}^{1d} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)P_0^B|x|^{-1}P_0^B\right)P_0^B - \left(1+\frac{\alpha}{2}\right)P_0^B.
\end{aligned}$$

Proof. The lemma follows from Lemma 6.1, Lemma 6.2, Lemma 6.3 and Lemma 6.4 in [**FG2015**].

$\square$

**Localization and decomposition.** In [**FG2015**] the authors decompose the mode space into $\mathcal{M}$ intervals, indexed with $b$, each of length $2\mathcal{K}_3/\mathcal{M}$ and consider for $u \in \mathbb{R}$ and $0 < \gamma < 1$ the block Hamiltonian

$$h_\gamma^{(u)} := \kappa_1 \left(-\partial_3^2\right) + \sum_b \left[ (1-\gamma) A_b^{(u)*} A_b^{(u)} + \frac{\sqrt{\alpha}}{2\pi} V(b) \left( A_b^{(u)} e^{ik_b x_3} + A_b^{(u)*} e^{-ik_b x_3} \right) \right]$$

with $k_b$ a mode in block $b$ and the block creation and annihlation operators $A_b^{(u)*}$ and $A_b^{(u)}$ acting on $\mathcal{F}\left(L^2\left(\mathbb{R}^3\right)\right)$, where

$$A_b^{(u)} := \frac{1}{V(b)} \int_b \nu\left(k_3\right) e^{i(k_3-k_b)u} \hat{a}_{k_3} dk_3$$

with $V(b) := \left(\int_b \nu\left(k_3\right)^2 dk_3\right)^{\frac{1}{2}}$. Furthermore

$$[A_b^{(u)}, A_{b'}^{(u)*}] = \delta_{bb'},\ [A_b^{(u)}, A_{b'}^{(u)}] = [A_b^{(u)*}, A_{b'}^{(u)*}] = 0 \ \text{ for all blocks } b, b'.$$

Lemma 22. *For $\chi \in C_0^\infty(\mathbb{R}), \|\chi\|_2 = 1$ a nonnegative function supported on the interval $[-1/2, 1/2]$ and for $J > 0$ denoting $\chi_u^J(x_3) = \sqrt{J}\chi\left(J^{-1}\left(x_3 - u\right)\right)$.*

$$\begin{aligned} &\mathfrak{h}^{1d} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right) P_0^B |x|^{-1} P_0^B \\ &\geq \int_{\mathbb{R}} \chi_u^J \left[h_\gamma^{(u)} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right) P_0^B |x|^{-1} P_0^B\right] \chi_u^J \, du - \frac{\alpha \mathcal{K}_3^2 J^2}{4\pi^2 \gamma \mathcal{M}^2} R - \|\chi'\|_2^2 J^{-2} \end{aligned}$$

*with*

$$R := \int_{|k_3| \leq \mathcal{K}_3} \nu\left(k_3\right)^2 dk_3 = \pi \int_{|k_3| \leq \mathcal{K}_3} \left(\ln\left(\mathcal{K}_\perp + k_3^2\right) - \ln\left(1 + k_3^2\right)\right) dk_3.$$

Proof. The lemma follows from Lemma 6.5 in [**FG2015**].

$\square$

**Error estimates.** Similarly as in [**FG2015**], [**Gh2012**] and [**LT1995**] representing the block creation and annihilation operators by coherent state integrals and completing the square it follows for a suitably chosen $k_b$ that

$$h_\gamma^{(u)} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right) P_0^B |x|^{-1} P_0^B \geq I - \mathcal{M}, \tag{4.3.1}$$

where

$$I = \inf_{\|\phi\|_2 = 1} \left[ \kappa_1 \|\partial_3 \phi\|_2^2 - \frac{\alpha}{4\pi^2(1-\gamma)} \int_{\mathbb{R}} \nu\left(k_3\right)^2 \left| \int_{\mathbb{R}^3} e^{ik_3 x_3} \left|\phi\left(x_\perp, x_3\right)\right|^2 dx \right|^2 dk_3 \right.$$
$$\left. - \frac{\beta}{1-\mathcal{A}^{-1}} \int_{\mathbb{R}^3} \frac{\left|\left(P_0^B \phi\right)\left(x_\perp, x_3\right)\right|^2}{|x|} dx \right]$$

Combining (4.3.1) with Lemma 22

$$\mathfrak{h}^{\mathrm{1d}} - \beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right) P_0^B |x|^{-1} P_0^B \geq I - \mathcal{M} - \frac{\alpha \mathcal{K}_3^2 J^2}{4\pi^2 \gamma \mathcal{M}^2} R - \|\chi'\|_2^2 J^{-2}.$$

Now it follows from Lemma 21 that for some constant $C>0$

$$P_0^B\left(\mathfrak{h}_{\mathcal{K}}^{\mathrm{co}}-\beta\left(1/\left(1-\mathcal{A}^{-1}\right)\right)|x|^{-1}\right)P_0^B$$
$$\geq \kappa B P_0^B+IP_0^B-C\left(\frac{\mathcal{K}_3 B}{\mathcal{K}_\perp^2}+\mathcal{M}+\frac{\mathcal{K}_3^2 J^2}{\gamma^2\mathcal{M}^2}R+\frac{1}{J^2}\right)P_0^B. \tag{4.3.2}$$

Lemma 23. *For any $L>0$ and $\epsilon>0$ and with $\mathcal{D}(B,L)$ as given in (4.1.1) assuming*

$$\frac{2\ln\mathcal{K}_\perp}{1-\gamma}=\frac{\mu(B)}{1-\mathcal{A}^{-1}}\quad \textit{and}\quad \tilde{\kappa}_1:=\kappa_1-\frac{4\beta\epsilon\,|\mathcal{D}(B,L)|\ln\mathcal{K}_\perp}{\mu(B)\,(1-\gamma)}>0 \tag{4.3.3}$$

*with $\mu(B):=\ln B-2\ln\ln B$,*

$$I\geq\frac{4\left(\ln\mathcal{K}_\perp\right)^2\mathfrak{e}_0}{\tilde{\kappa}_1\left(1-\gamma\right)^2}-\frac{2\beta\ln\mathcal{K}_\perp}{\mu(B)\,(1-\gamma)}\left(\frac{432L^2}{|\mathcal{D}(B,L)|^3\epsilon^3}+\frac{1}{L}+\frac{|\mathcal{D}(B,L)|}{\epsilon}\right).$$

Proof. For $\phi\in L^2\left(\mathbb{R}^3\right)$, $\|\phi\|_2=1$ denoting

$$\tilde{\phi}(x_3):=\left(\int_{\mathbb{R}^2}|\phi\left(x_\perp,x_3\right)|^2dx_\perp\right)^{\frac{1}{2}},$$

$$\begin{aligned}
&\kappa_1\|\partial_3\phi\|_2^2-\frac{\alpha}{4\pi^2\left(1-\gamma\right)}\int_{\mathbb{R}}\nu\left(k_3\right)^2\left|\int_{\mathbb{R}^3}e^{ik_3x_3}\left|\phi\left(x_\perp,x_3\right)\right|^2dx\right|^2dk_3\\
&\quad-\frac{\beta}{1-\mathcal{A}^{-1}}\int_{\mathbb{R}^3}\frac{\left|\left(P_0^B\phi\right)\left(x_\perp,x_3\right)\right|^2}{|x|}dx\\
&\geq\kappa_1\|\partial_3\phi\|_2^2-\frac{\alpha\ln\mathcal{K}_\perp}{1-\gamma}\int_{\mathbb{R}}\left|\int_{\mathbb{R}^2}\left|\phi\left(x_\perp,x_3\right)\right|^2dx_\perp\right|^2dx_3\\
&\quad-\frac{\beta}{1-\mathcal{A}^{-1}}\int_{\mathbb{R}^3}\frac{\left|\left(P_0^B\phi\right)\left(x_\perp,x_3\right)\right|^2}{|x|}dx\\
&\geq\left(\kappa_1-\frac{2\beta\epsilon\,|\mathcal{D}(B,L)|}{1-\mathcal{A}^{-1}}\right)\|\partial_3\tilde{\phi}\|_2^2-\frac{\alpha\ln\mathcal{K}_\perp}{1-\gamma}\|\tilde{\phi}\|_4^4-\frac{\beta\mu(B)}{1-\mathcal{A}^{-1}}\left(\tilde{\phi}(0)\right)^2\\
&\quad-\frac{\beta}{1-\mathcal{A}^{-1}}\left(\frac{432L^2}{|\mathcal{D}(B,L)|^3\epsilon^3}+\frac{1}{L}+\frac{|\mathcal{D}(B,L)|}{\epsilon}\right)\\
&\geq\frac{4\left(\ln\mathcal{K}_\perp\right)^2\mathfrak{e}_0}{\tilde{\kappa}_1\left(1-\gamma\right)^2}-\frac{2\beta\ln\mathcal{K}_\perp}{\mu(B)\,(1-\gamma)}\left(\frac{432L^2}{|\mathcal{D}(B,L)|^3\epsilon^3}+\frac{1}{L}+\frac{|\mathcal{D}(B,L)|}{\epsilon}\right).
\end{aligned}$$

At the first inequality it is used that

$$\nu\left(k_3\right)^2=\pi\left(\ln\left(\mathcal{K}_\perp^2+k_3^2\right)-\ln\left(1+k_3^2\right)\right)\leq 2\pi\ln\mathcal{K}_\perp \tag{4.3.4}$$

along with Plancherel's identity. At the second inequality the bathtub principle in Lemma 12 and the argument in the proof of Corollary 14 apply mutatis mutandis. At the third inequality the assumptions in (4.3.3) are used.

□

From Lemma 23 and further assuming

$$\kappa-\tilde{\kappa}_1\leq\frac{\kappa}{2}\quad\text{and}\quad\gamma\leq\frac{1}{2}, \tag{4.3.5}$$

it can be seen there is a constant $C > 0$ such that

$$I \geq 4\kappa^{-1} (\ln \mathcal{K}_\perp)^2 \mathfrak{e}_0 - C \left( \frac{(\ln \mathcal{K}_\perp)^2}{\kappa} \left( \frac{\kappa - \tilde{\kappa}_1}{\kappa} + \gamma \right) + \frac{\ln \mathcal{K}_\perp}{\mu(B)} \left( \frac{L^2}{|\mathcal{D}(B,L)|^3 \epsilon^3} + \frac{1}{L} + \frac{|\mathcal{D}(B,L)|}{\epsilon} \right) \right).$$

With the above bound and (4.3.2) the argument in [**FG2015**] applies mutatis mutandis and choosing $J^2 = \kappa^{1/5} \mathcal{K}_3^{-3/5} (\ln \mathcal{K}_\perp)^{-3/5}$, $\mathcal{M} = [J^{-2}]$ and $\gamma = \kappa^{4/5} \mathcal{K}_3^{3/5} (\ln \mathcal{K}_\perp)^{-7/5}$ yields

$$\begin{aligned} &P_0^B \left( \mathfrak{h}_{\mathcal{K}}^{\mathrm{co}} - \beta \left( 1/\left(1 - \mathcal{A}^{-1}\right)\right) |x|^{-1} \right) P_0^B \\ &\geq \left( \kappa B + \frac{4 (\ln \mathcal{K}_\perp)^2}{\kappa} \mathfrak{e}_0 \right) P_0^B \\ &\quad - C \left( \kappa^{-1} (\kappa - \kappa_1) (\ln \mathcal{K}_\perp)^2 + \kappa^{-1/5} \mathcal{K}_3^{3/5} (\ln \mathcal{K}_\perp)^{3/5} + B \mathcal{K}_3 \mathcal{K}_\perp^{-2} \right) P_0^B \\ &\quad - C \frac{\ln \mathcal{K}_\perp}{\mu(B)} \left( \frac{L^2 \epsilon^{-3}}{|\mathcal{D}(B,L)|^3} + \frac{1}{L} + \frac{|\mathcal{D}(B,L)|}{\epsilon} + \frac{\epsilon |\mathcal{D}(B,L)| (\ln \mathcal{K}_\perp)^2}{\kappa} \right) P_0^B. \end{aligned}$$

It is shown in [**FG2015**] choosing $\mathcal{K}_\perp = B^{1/2}$ and $\mathcal{K}_3 = \kappa^{-1/2} (\ln B)^{3/2}$

$$\kappa^{-1} (\kappa - \kappa_1) (\ln \mathcal{K}_\perp)^2 + \kappa^{-1/5} \mathcal{K}_3^{3/5} (\ln \mathcal{K}_\perp)^{3/5} + B \mathcal{K}_3 \mathcal{K}_\perp^{-2} \leq C \kappa^{-1/2} (\ln B)^{3/2}.$$

Now choosing $L = (\ln B)^{-1}$ and $\epsilon = (\ln B)^{-1}$ since $1 \leq |\mathcal{D}(B,L)| \leq C$ for $B \geq C$

$$\frac{\ln \mathcal{K}_\perp}{\mu(B)} \left( \frac{L^2 \epsilon^{-3}}{|\mathcal{D}(B,L)|^3} + \frac{1}{L} + \frac{|\mathcal{D}(B,L)|}{\epsilon} + \frac{\epsilon |\mathcal{D}(B,L)| (\ln \mathcal{K}_\perp)^2}{\kappa} \right) \leq C \left(1 + \kappa^{-1}\right) \ln B.$$

With the above choice of parameters and the assumptions $C (\ln B)^{-1/2} \leq \kappa \leq C^{-1} \ln B$ and $\mathcal{K} \geq \sqrt{B}$, the conditions in (4.3.3) and (4.3.5) and that $0 < \mathcal{K}_3 \leq \mathcal{K}$ , $1 \leq \mathcal{K}_\perp \leq \mathcal{K}$ and $1 < \mathcal{A} < (B/\ln B)^{1/2}$ are verified, and

$$\begin{aligned} &P_0^B \left( \mathfrak{h}_{\mathcal{K}}^{\mathrm{co}} - \beta \left( 1/\left(1 - \mathcal{A}^{-1}\right)\right) |x|^{-1} \right) P_0^B \\ &\geq \left( \kappa B + \kappa^{-1} (\ln B)^2 \mathfrak{e}_0 - C \kappa^{-1/2} (\ln B)^{3/2} - C \left(1 + \kappa^{-1}\right) \ln B \right) P_0^B. \end{aligned}$$

Corollary 24. *For $W$ a sum of a bounded Borel measure on the real line and a $L^\infty(\mathbb{R})$-function, $E_\epsilon(B)$ the ground-state energy of the perturbed Hamiltonian in (1.2.10) and $\mathfrak{e}_\epsilon$ as given in (1.2.12) there is a constant $C > 0$ such that for $B > 1$*

$$E_\epsilon(B) \geq B + \mathfrak{e}_\epsilon (\ln B)^2 - C (\ln B)^{3/2}.$$

Proof. Since $W$ is a one-dimensional perturbation, the above proof strategy remains unchanged.

□

### 4.4. Proof of Theorem 2

Proof. Let $E_\epsilon(B)$ be the ground-state energy of the perturbed Hamiltonian $\mathbb{H}_\epsilon(B)$ in (1.2.10) and let the one-dimensional energy $\mathfrak{e}_\epsilon$ be as defined in (1.2.12). By Corollary 10 and

Corollary 24,

$$\lim_{B\to\infty}\frac{E_\epsilon(B)-B}{(\ln B)^2}=\mathfrak{e}_\epsilon. \tag{4.4.1}$$

As explained in the introduction, it follows from the variational principle, Theorem 1 and (4.4.1) that for $\epsilon>0$

$$\frac{\mathfrak{e}_0-\mathfrak{e}_\epsilon}{\epsilon}\geq\limsup_{B\to\infty}\frac{1}{(\ln B)}\int_{\mathbb{R}}W(x_3)\left(\int_{\mathbb{R}^2}\left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2\left(x_{\perp,\frac{x_3}{(\ln B)}}\right)dx_\perp\right)dx_3$$

and, when $\epsilon<0$ ,

$$\frac{\mathfrak{e}_0-\mathfrak{e}_\epsilon}{\epsilon}\leq\liminf_{B\to\infty}\frac{1}{(\ln B)}\int_{\mathbb{R}}W(x_3)\left(\int_{\mathbb{R}^2}\left\|\Psi^{(B)}\right\|_{\mathcal{F}}^2\left(x_{\perp,\frac{x_3}{(\ln B)}}\right)dx_\perp\right)dx_3.$$

Theorem 2 now follows from Theorem 6.

□

**A Remark on the One-Dimensional Strong-Coupling Polaron.** The proof of the lower bound relies on an argument of Frank and Geisinger, who rely on a one-dimensional version of the Lieb-Thomas proof. This will explained here generically for a one-dimensional bound polaron.

$$H_\alpha(V)=p^2+\sum_k a_k^\dagger a_k-\left(\frac{\alpha}{L}\right)^{\frac{1}{2}}\sum_k\left(a_ke^{ikx}+a_k^\dagger e^{-ikx}\right)-\alpha^2V(\alpha x)$$

defined now on $\mathcal{F}\otimes L^2(\mathbb{R})$, where $\mathcal{F}$ is a symmetric Fock space over $\ell^2(\mathbb{Z}/L)$. The length of the crystal is $2L$ and the lattice spacing is $1/L$. (The continuum approximation $\sum_k\to L\int dk$ is valid for the model.) The arguments apply also when $V\equiv 0$; the external potential needs to be scaled with the electron-phonon coupling parameter for its effect to survive in the strong-coupling limit (as explained in Introduction of thesis). The ground-state energy is $E_\alpha(V)$. It follows using a product state with an electronic wave function and a coherent state, as above, that $E_\alpha(V)\leq\alpha^2e(V)$, where $e(V)$ is the following one-dimensional minimization problem:

$$e(V):=\inf_{\|\varphi\|_{L^2(\mathbb{R})}=1}\left\{\int_{\mathbb{R}}|\varphi'|^2\,dx-\alpha\int_{\mathbb{R}}|\varphi|^4\,dx-\int_{\mathbb{R}}V(x)\,|\varphi(x)|^2\,dx\right\}.$$

It will be illustrated here in full detail how to arrive at an agreeable lower bound to establish $\lim\limits_{\alpha\to\infty}\frac{E_\alpha(V)}{\alpha^2}=e(V)$. (Recall: In the one-dimensional problem treated above, the electron-phonon interaction was $\alpha\ln B$ and were were taking the limit $B\to\infty$. Here I just take $\alpha\to\infty$ for ease of notation and also not use any unnecessary parameters in order to illustrate as clearly as possible the lower bound.

*Ultraviolet Cutoff.* We ignore large modes in the Fröhlich Hamiltonian and work on a reduced mode space $\{k:\ |k|\leq K\}$ with a cutoff Hamiltonian

$$H_K=(1-\epsilon)p^2+\sum_{|k|\leq K}a_k^\dagger a_k-\left(\frac{\alpha}{L}\right)^{\frac{1}{2}}\sum_{|k|\leq K}\left(a_ke^{ikx}+a_k^\dagger e^{-ikx}\right)-\alpha^2V(\alpha x) \tag{4.4.2}$$

The parameters $\epsilon$ and $K$ will be chosen at the very end of the computations.

We bound the energy of the Fröhlich Hamiltonian from below with the energy of the *cutoff Hamiltonian* $H_K$ in (4.4.2). We observe

$$H_\alpha(V) = H_K + \epsilon p^2 + \sum_{|k|>K} a_k^\dagger a_k - \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k|>K} \left(a_k e^{ikx} + a_k^\dagger e^{-ikx}\right) \tag{4.4.3}$$

and we will arrive at a lower bound by making an estimate on the interaction term in (4.4.3).

We use a standard commutator identity $\langle [p, a_k e^{ikx}] \rangle = k \langle a_k e^{ikx} \rangle$ and work with two operators $Z = \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k|>K} \frac{a_k e^{ikx}}{k}$ and $Z^\dagger = \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k|>K} \frac{a_k^\dagger e^{-ikx}}{k}$.

For any $0 < \epsilon < 1$,

$$\begin{aligned}
\left\langle \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{|k|>K} \left(a_k e^{ikx} + a_k^\dagger e^{-ikx}\right) \right\rangle &= \left\langle [p, Z - Z^\dagger] \right\rangle \\
&\leq 2 \left\langle p^2 \right\rangle^{\frac{1}{2}} \left\langle -(Z - Z^\dagger)^2 \right\rangle^{\frac{1}{2}} \\
&\leq \epsilon \left\langle p^2 \right\rangle + \frac{1}{\epsilon} \left\langle -(Z - Z^\dagger)^2 \right\rangle \\
&\leq \epsilon \left\langle p^2 \right\rangle + \frac{2}{\epsilon} \left\langle Z Z^\dagger + Z^\dagger Z \right\rangle \qquad (4.4.4) \\
&= \epsilon \left\langle p^2 \right\rangle + \frac{2}{\epsilon} \left\langle [Z, Z^\dagger] \right\rangle + \frac{4}{\epsilon} \left\langle Z^\dagger Z \right\rangle \\
&\leq \epsilon \left\langle p^2 \right\rangle + \frac{4\alpha}{\epsilon K} + \frac{8\alpha}{\epsilon K} \left\langle \sum_{|k|>K} a_k^\dagger a_k \right\rangle \qquad (4.4.5)
\end{aligned}$$

Above, (4.4.4) is immediate from the positive definiteness of $(Z + Z^\dagger)^2$. To arrive at (4.4.5), we make the following estimates on $\langle Z^\dagger Z \rangle$ and $\langle [Z, Z^\dagger] \rangle$:

$$\begin{aligned}
\left\langle Z^\dagger Z \right\rangle &= \left(\frac{\alpha}{L}\right) \sum_{|k|>K} \sum_{|k'|>K} \left\langle \frac{a_k^\dagger a_{k'} e^{i(k'-k)x}}{k k'} \right\rangle \\
&\leq \left(\frac{\alpha}{L}\right) \left( \sum_{|k|>K} \frac{1}{k} \langle a_k^\dagger a_k \rangle^{\frac{1}{2}} \right)^2 \\
&\leq \left(\frac{\alpha}{L}\right) \left( \sum_{|k|>K} \frac{1}{|k|^2} \right) \left( \sum_{|k|>K} \langle a_k^\dagger a_k \rangle \right) \\
&\leq \frac{2\alpha}{K} \left\langle \sum_{|k|>K} a_k^\dagger a_k \right\rangle
\end{aligned}$$

Since $[a_k, a_{k'}^\dagger] = \delta_{kk'}$,

$$\left\langle [Z, Z^\dagger] \right\rangle = \left(\frac{\alpha}{L}\right) \sum_{|k|>K} \sum_{|k'|>K} \left\langle \frac{e^{i(k-k')x}(a_k a_{k'}^\dagger - a_{k'}^\dagger a_k)}{k k'} \right\rangle$$

$$\leq \left\langle \frac{2\alpha}{K} \right\rangle$$

We can now construct a lower bound from (4.4.3):

$$\langle H_\alpha(V)\rangle \geq \langle H_K\rangle + \left(1 - \frac{8\alpha}{\epsilon K}\right)\left\langle \sum_{|k|>K} a_k^\dagger a_k \right\rangle - \left\langle \frac{4\alpha}{\epsilon K}\right\rangle$$

Clearly, we require from our parameters $\epsilon$ and $K$ that $1 = \frac{8\alpha}{\epsilon K}$. We now arrive at our lower bound:

$$E_\alpha(V) \geq \inf_{\|\Psi\|=1} \langle \Psi,\ H_K\Psi\rangle - \frac{1}{2}.$$

In sharp contrast to the three-dimensional computation performed in [LiTh], our error term, $-\frac{1}{2}$, does not depend on the cutoff parameter $K$.

*Localizing the Electron.* We will bound *from below* the ground state energy of the cutoff Hamiltonian $H_K$: $\inf\limits_{\|\Psi\|=1} \langle \Psi,\ H_k\Psi\rangle$ (given in (4.4.2)).

Here, $(\triangle E) > 0$ is a parameter whose specific value will be given at the very end of the computations. We will denote by $\inf\limits_{\|\Psi\|}{}' \langle \Psi,\ H_K\Psi\rangle$ the infimum taken over all wave functions whose *electronic coordinate is localized* in an interval of length $\frac{\pi}{(\triangle E)^{\frac{1}{2}}}$. This restriction, we argue, increases the ground state energy of $H_K$ by atmost $\triangle E$:

$$\inf_{\|\Psi\|=1} \langle \Psi,\ H_K\Psi\rangle \geq \inf_{\|\Psi\|=1}{}' \langle \Psi,\ H_K\Psi\rangle - (\triangle E) \tag{4.4.6}$$

Let $\|\Psi\| = 1$ and $E = \langle \Psi,\ H_K\Psi\rangle$. We define $\phi(x) = \cos\left((\triangle E)^{\frac{1}{2}}x\right)$ on its support in $\left(-\frac{\pi}{2(\triangle E)^{\frac{1}{2}}}, \frac{\pi}{2(\triangle E)^{\frac{1}{2}}}\right)$ and write $\phi_y(x) = \phi(x-y)$. To argue (4.4.6), it suffices to show for some $\bar{y} \in \mathbb{R}$,

$$\frac{\langle (\phi_{\bar{y}}\Psi)\,,\ H_K\,(\phi_{\bar{y}}\Psi)\rangle}{\langle \phi_{\bar{y}}\Psi,\ \phi_{\bar{y}}\Psi\rangle} \leq E + (\triangle E). \tag{4.4.7}$$

A direct calculation gives $\int_{\mathbb{R}} \langle (\phi_y\Psi)\,,\ H_K\,(\phi_y\Psi)\rangle\, dy = \int (\phi')^2 + E\phi^2 dx$ and

$$\int_{\mathbb{R}} \left(\langle (\phi_y\Psi)\,,\ H_K\,(\phi_y\Psi)\rangle - (E + \triangle E)\,\langle \phi_y\Psi,\ \phi_y\Psi\rangle\right) dy$$

$$= \int_{-\frac{\pi}{2(\triangle E)^{\frac{1}{2}}}}^{\frac{\pi}{2(\triangle E)^{\frac{1}{2}}}} (\phi')^2 - (\triangle E)\phi^2 dx = 0$$

since $(\triangle E)$ is the Dirichlet energy of $\phi$. So there exists some $\bar{y} \in \mathbb{R}$ such that (4.4.7) holds. From now on, we consider the electron to be localized in some interval of length $\frac{\pi}{(\triangle E)^{\frac{1}{2}}}$.

*Block Hamiltonian.* We now decompose our finite mode space into finitely many blocks: $\{k :\ |k| < K\} = \bigcup\limits_n \{B_n\}$; each block $B_n$ contains "$PL$" modes where "$\max\limits_{k_i,k_j \in B_n} |k_i - k_j| = P$" is the size of each block.

On each block $B_n$ we analogously define block annihlation and creation operators: $A_{B_n} = \frac{1}{(PL)^{\frac{1}{2}}} \sum\limits_{k\in B_n} a_k$ and $A_{B_n}^\dagger = \frac{1}{(PL)^{\frac{1}{2}}} \sum\limits_{k\in B_n} a_k^\dagger$. Clearly, $[A_{B_m}, A_{B_n}^\dagger] = \delta_{mn}$. On each block $B_n$, we see from the Cauchy-Schwarz inequality that

$$A_{B_n}^{\dagger} A_{B_n} \le \sum_{k\in B_n} a_k^{\dagger} a_k. \tag{4.4.8}$$

For reasons that will become clear in the next stage of the computation, we now want to work with the approximation that the electron interacts with atmost one mode $k_{B_n}$ in each block $B_n$. For this approximation to work, we make the following estimate on the interaction term of our cutoff Hamiltonian: for any parameter $0 < \delta < 1$ and any mode $k_{B_n}$ in each block $B_n$, completing the square yields

$$\begin{aligned}
&\left\langle \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{B_n} \sum_{k\in B_n} \left[a_k \left(e^{ik_{B_n}x} - e^{ikx}\right) + a_k^{\dagger}\left(e^{-ik_{B_n}x} - e^{-ikx}\right)\right] \right\rangle \\
&\le \left\langle \delta \sum_{|k|<K} a_k^{\dagger} a_k + \left(\frac{\alpha}{L}\right)\frac{1}{\delta} \sum_{B_n}\sum_{k\in B_n} \left|e^{ik_{B_n}x} - e^{ikx}\right|^2 \right\rangle \\
&\le \left\langle \delta \sum_{|k|<K} a_k^{\dagger} a_k + \left(\frac{\alpha}{L}\right)\frac{1}{\delta} \sum_{B_n}\sum_{k\in B_n} |k - k_{B_n}|^2 |x|^2 \right\rangle \\
&\le \left\langle \delta \sum_{|k|<K} a_k^{\dagger} a_k \right\rangle + \frac{2\alpha K P^2 \pi^2}{\delta(\triangle E)}. 
\end{aligned} \tag{4.4.9}$$

To arrive at (4.4.9), we used the rigorously justified approximation (see (4.4.6)) that the electronic co-ordinate is localized in an interval of length $\frac{\pi}{(\triangle E)^{\frac{1}{2}}}$.

The parameters $P$ and $0 < \delta < 1$ will be chosen at the very end of the computations; the specific mode $k_{B_n}$ in each block will be chosen in the next stage of the computation.

Now we bound the ground state energy of the cutoff Hamiltonian (with the condition that the electronic co-ordinate of the ground-state wave function is localized) $\inf_{\|\Psi\|=1}{}' \langle \Psi,\ H_K \Psi\rangle$, from below, using the energy of the *block Hamiltonian*:

$$\begin{aligned}
&H_K^{\text{Block}}(\{k_{B_n}\}) \\
&= (1-\epsilon)p^2 + (1-\delta)\sum_{B_n} A_{B_n}^{\dagger} A_{B_n} - (P\alpha)^{\frac{1}{2}} \sum_{B_n} \left(A_{B_n} e^{ik_{B_n}x} + A_{B_n}^{\dagger} e^{-ik_{B_n}x}\right) - \alpha^2 V(\alpha x).
\end{aligned} \tag{4.4.10}$$

Clearly,

$$\begin{aligned}
H_K = &\Bigg( (1-\epsilon)p^2 + \sum_{|k|<K} a_k^{\dagger} a_k - \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{B_n}\sum_{k\in B_n} \left(a_k e^{ik_{B_n}x} + a_k^{\dagger} e^{-ik_{B_n}x}\right) + \\
&-\alpha^2 V(\alpha x) + \left(\frac{\alpha}{L}\right)^{\frac{1}{2}} \sum_{B_n}\sum_{k\in B_n} \left[a_k\left(e^{ik_{B_n}x} - e^{ikx}\right) + a_k^{\dagger}\left(e^{-ik_{B_n}x} - e^{-ikx}\right)\right] \Bigg) \\
&\ge H_K^{\text{Block}}(\{k_{B_n}\}) - \frac{2\alpha K P^2 \pi^2}{\delta(\triangle E)},
\end{aligned} \tag{4.4.11}$$

in the sense of expectation values. To arrive at (4.4.11) we simply used the estimates from (4.4.8) and (4.4.9).

We summarize:

$$\inf_{\|\Psi\|=1}{}' \langle\Psi,\ H_K\Psi\rangle \geq \inf_{\|\Psi\|=1}{}' \sup_{\{k_{B_n}\}} \left\langle \Psi,\ H_K^{\text{Block}}\left(\{k_{B_n}\}\right)\Psi\right\rangle - \frac{2\alpha K P^2\pi^2}{\delta(\triangle E)}.$$

*Coherent States.* We now work with the block Hamiltonian $H_K^{\text{Block}}\left(\{k_{B_n}\}\right)$ from (4.4.10) and the block creation and annihlation operators constructed in the previous stage of the computation. For each block $B_n$ we define a block coherent state indexed by some $z_{B_n}\in\mathbb{C}$:

$$|z_{B_n}\rangle = \pi^{-\frac{1}{2}}\left(e^{-\frac{|z_{B_n}|^2}{2}+z_{B_n}A^\dagger_{B_n}}\right)|0_{B_n}\rangle\,,$$

where $|0_{B_n}\rangle$ denotes the vacuum state in block $B_n$, i.e., $A_{B_n}|0_{B_n}\rangle = 0$. We write

$$|z\rangle = \prod_{B_n}|z_{B_n}\rangle\,,$$

a tensor product of the coherent states corresponding to each block $B_n$.

One can verify that for each block $B_n$, the coherent state $|z_{B_n}\rangle$ is the eigenstate of the corresponding block annihlation operator:

$$A_{B_n}|z_{B_n}\rangle = z_{B_n}|z_{B_n}\rangle\,.$$

The commutator relation $[A_{B_m},A^\dagger_{B_n}]=\delta_{mn}$, together with the resolution of identity formula

$$I=\int |z\rangle\langle z|\prod_{B_m} dz_{B_m}d\overline{z_{B_m}},$$

yield the convenient representations:

$$A_{B_n}=\int z_{B_n}|z\rangle\langle z|\prod_{B_m} dz_{B_m}d\overline{z_{B_m}}$$

$$A^\dagger_{B_n}A_{B_n}=\int\left(|z_{B_n}|^2-1\right)|z\rangle\langle z|\prod_{B_m} dz_{B_m}d\overline{z_{B_m}}$$

Denoting $\Psi_z(x)=\langle z\mid\Psi\rangle_{\text{Phonon}}$(the inner product only in the phonon coordinates), we recast the energy of the block Hamiltonian $H_K^{\text{Block}}\left(\{k_{B_n}\}\right)$ in the following form:

$$\left\langle\Psi,\ H_K^{\text{Block}}\left(\{k_{B_n}\}\right)\Psi\right\rangle = \int\langle\Psi_z,\ h_z\Psi_z\rangle_{\text{E}}\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} \tag{4.4.12}$$

where $\langle\cdot,\cdot\rangle_{\text{E}}$ is the inner product only over the electronic coordinate, and $h_z$ is the Schrödinger operator:

(4.4.13)

$$h_z=(1-\epsilon)p^2+\sum_{B_n}\left[(1-\delta)\left(|z_{B_n}|^2-1\right)-(P\alpha)^{\frac{1}{2}}\left(z_{B_n}e^{ik_{B_n}x}+\overline{z_{B_n}}e^{-ik_{B_n}x}\right)\right]-\alpha^2V(\alpha x)$$

Since

$$\left(\langle\Psi_z,\Psi_z\rangle_E(1-\delta)\overline{z_{B_n}}-(P\alpha)^{\frac{1}{2}}\langle\Psi_z,e^{ik_{B_n}x}\Psi_z\rangle_E\right)\left(z_{B_n}-\frac{(P\alpha)^{\frac{1}{2}}}{(1-\delta)\langle\Psi_z,\Psi_z\rangle}\langle\Psi_z,e^{-ik_{B_n}x}\Psi_z\rangle_E\right)\geq 0,$$

completing the square yields

$$(1-\delta)\langle\Psi_z,\Psi_z\rangle_E|z_{B_n}|^2-\overline{z_{B_n}}(P\alpha)^{\frac{1}{2}}\langle\Psi_z,e^{-ik_{B_n}x}\Psi_z\rangle_E-z_{B_n}(P\alpha)^{\frac{1}{2}}\langle\Psi_z,e^{ik_{B_n}x}\Psi_z\rangle_E$$

$$\geq \frac{-(P\alpha)\left|\langle\Psi_z, e^{-ik_{B_n}x}\Psi_z\rangle_E\right|^2}{(1-\delta)\langle\Psi_z,\Psi_z\rangle_E}.$$

The advantage of constructing a Block Hamiltonian in the previous subsection is that the energy error we incur for disregarding the "-1" term in (4.4.13) is proportional to the number of blocks: $\frac{2K}{P}$, a finite value.

In the following calculation, in each block $B_n$ we choose a mode $\mathcal{K}_{\mathbf{B_n}}$ such that

$$\left|\langle\Psi_z, e^{-i\mathcal{K}_{\mathbf{B_n}}x}\Psi_z\rangle_E\right|^2 = \min_{k\in B_n}\left|\langle\Psi_z, e^{-ikx}\Psi_z\rangle_E\right|^2.$$

As seen in (4.4.16) below, we also make use of the continuum approximation $\sum_k \to L\int dk$ permitted by our model. We now proceed to extract the Pekar energy functional from (4.4.12):

$$\sup_{\{k_{B_n}\}}\left\langle\Psi,\ H_K^{\text{Block}}\left(\{k_{B_n}\}\right)\Psi\right\rangle$$

$$\begin{aligned}
\text{(4.4.14)}\qquad &\geq \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times\left((1-\epsilon)\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha P}{(1-\delta)}\sum_{B_n}\frac{\left|\left\langle\Psi_z,\ e^{-i\mathcal{K}_{\mathbf{B_n}}x}\Psi_z\right\rangle_{\mathrm{E}}\right|^2}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}+\right.\\
&\left.-\alpha^2\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}\\
&= \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times\left((1-\epsilon)\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha}{(1-\delta)}\frac{1}{L}\sum_{B_n}\frac{(PL)\left|\left\langle\Psi_z,\ e^{-i\mathcal{K}_{\mathbf{B_n}}x}\Psi_z\right\rangle_{\mathrm{E}}\right|^2}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}+\right.\\
&\left.-\alpha^2\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}\\
\text{(4.4.15)}\qquad &\geq \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times\left((1-\epsilon)\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha}{(1-\delta)}\frac{1}{L}\sum_{k}\frac{\left|\left\langle\Psi_z,\ e^{-ikx}\Psi_z\right\rangle_{\mathrm{E}}\right|}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}+\right.\\
&\left.-\alpha^2\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}\\
\text{(4.4.16)}\qquad &= \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times\left((1-\epsilon)\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha}{(1-\delta)}\int\left(\frac{\left|\left\langle\Psi_z,\ e^{-ikx}\Psi_z\right\rangle_{\mathrm{E}}\right|^2}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}\right)dk+\right.\\
&\left.-\alpha^2\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}\\
\text{(4.4.17)}\qquad &= \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times\left((1-\epsilon)\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha}{(1-\delta)}\int\left(\frac{|\Psi_z|^4}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}\right)dx+\right.\\
&\left.-\alpha^2\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}\\
&\geq \int\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\times(1-\epsilon)\left(\frac{\left\langle\Psi_z,\ p^2\Psi_z\right\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}} - \frac{\alpha}{(1-\delta)(1-\epsilon)}\int\left(\frac{|\Psi_z|^4}{\left|\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}\right|^2}\right)dx+\right.\\
&\left.-\frac{\alpha^2}{(1-\epsilon)^2(1-\delta)^2}\frac{\langle\Psi_z,\ V(\alpha x)\Psi_z\rangle_{\mathrm{E}}}{\langle\Psi_z,\ \Psi_z\rangle_{\mathrm{E}}}\right)\prod_{B_m}dz_{B_m}d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P}
\end{aligned}$$

$$\geq \int \langle \Psi_z,\ \Psi_z \rangle_{\mathrm{E}} \left( \frac{\alpha^2 e(V)}{(1-\epsilon)(1-\delta)^2} \right) \prod_{B_m} dz_{B_m} d\overline{z_{B_m}} - (1-\delta)\frac{2K}{P} \tag{4.4.18}$$

$$= \frac{\alpha^2 e(V)}{(1-\epsilon)(1-\delta)^2} - (1-\delta)\frac{2K}{P},$$

where $e(V)$ is the Pekar energy, defined in (4.4.2). Above (4.4.17) follows from the Plancherel's theorem, and (4.4.18) follows from the scaling properties of our Pekar functional.

*Controlling the Error Terms.* We have the following upper and lower bounds on the ground-state energy:

$$\alpha^2 e(V) \geq E_\alpha(V) \geq \frac{e(V)\alpha^2}{(1-\epsilon)(1-\delta)^2} - (1-\delta)\frac{2K}{P} - \frac{1}{2} - (\triangle E) - \frac{2\alpha K P^2 \pi^2}{\delta(\triangle E)} \tag{4.4.19}$$

$$= \alpha^2 e(V) - \underbrace{\left( \left( \frac{\alpha^2\delta^2 - 2\alpha^2\delta - \frac{8\alpha^3}{K} + \frac{16\alpha^3\delta}{K} - \frac{8\alpha^3\delta^2}{K}}{1 - 2\delta + \delta^2 - \frac{8\alpha}{K} + \frac{16\alpha\delta}{K} - \frac{8\alpha\delta^2}{K}} \right) e(V) - (1-\delta)\frac{2K}{P} - \frac{1}{2} - (\triangle E) - \frac{2\alpha K P^2\pi^2}{\delta(\triangle E)} \right)}_{\text{error-term}},$$

since we noted, when using an ultraviolet cutoff above, that the parameters $\epsilon$ and $K$ must satisfy the coupling relation: $\epsilon = \frac{8\alpha}{K}$. We now choose specific values (in orders of $\alpha$) for the parameters $K, \delta, P$ and $\triangle E$ so that the error-term above is of an order less than $\alpha^2$, while satisfying the following constraints: $0 < \delta < 1$ and $P < K$ when $\alpha \gg 1$. In an attempt to make the error-term as small as possible, we have chosen

$$\delta = c_1\alpha^{-\frac{1}{7}}, K = c_2\alpha^{\frac{76}{49}}, P = c_3\alpha^{\frac{5}{49}} \text{ and } \triangle E = c_4\alpha^{\frac{64}{49}}.$$

From (4.4.19) we conclude

$$\alpha^2 e(V) \geq E_\alpha(V) \geq \alpha^2 e(V) - C\alpha^{\frac{71}{49}}.$$

CHAPTER 5

# Some Remarks about the Strong-Coupling Limit

He we will showcase a discrepancy in spherical symmetry between a rotation-invariant Hamiltonian and its unique ground state on the one hand and the corresponding Pekar Ansatz for the wave function on the other. To our knowledge, this will be the first demonstration of such an inconsistency concerning Pekar's Ansatz for a polaron localized in some external potential. However, our interest in the Ansatz in regard to the ground-state symmetry of the polaron is not new; on the contrary, this is a rather old and contentious topic that has attracted sizeable attention over the years, but until now only in the context of the translation-invariant (TI-) polaron. Indeed, some of the earliest enduring criticisms of Pekar's effective theory– notwithstanding its success at approximating the ground-state energy (in a certain regime)– stem from the fact that his Ansatz for the TI-polaron is a *localized* wave function, which clearly does not share the translational symmetry of the corresponding Hamiltonian. Moreover, this analogous discrepancy in translational symmetry was at the heart of a six-decades-long debate on whether an electron can be trapped in a phonon hole of its own making. (It is now known that the ground state of the TI-polaron is *delocalized* and that the aforementioned self-localization is merely an artifact of Pekar's Ansatz.) Therefore, starting as early as 1949 with the work of N.N. Bogoliubov and S.V. Tyablikov, for example, there have been many attempts to modify Pekar's Ansatz for the TI-polaron in order to restore the much-needed translational symmetry to Pekar's theory. But it remains to understand rigorously how these modified Ansätze for the TI-polaron are related to the (translation-invariant) ground state of the zero-momentum fiber Hamiltonian (cf. a recent exciting conjecture of Lieb and R. Seiringer discussed in the introduction of the thesis). Fortunately, the situation is somewhat more tractable for the example we shall provide in this paper, however unsettling it is to see that the corresponding Pekar Ansatz lacks the rotational invariance of the true ground-state wave function. To our surprise–and unlike for the analogous TI-polaron discussed above– we shall iron out this apparent contradiction in spherical symmetry under the assumption that the corresponding nonradial minimizers in Pekar's problem are unique up to a rotation. We shall also provide a conjecture for the general case where the minimizers are not necessarily unique up to a rotation.

Having outlined our vision for the polaron ground state, we now describe in detail the Fröhlich polaron localized in an external electric potential. As a model of an electron bound to an impurity in a polar crystal, it has received considerable attention (e.g. [**BP1957**], [**Pz1961**] and [**Ad1985**]; in the mathematical physics literature see [**Sp1986**], [**Lw1988a**] and [**Lw1988b**] about the existence of a pinning transition). The corresponding Fröhlich Hamiltonian is

$$H_\alpha^V = \mathbf{p}^2 - \alpha^2 V(\alpha x) + \int_{\mathbb{R}^3} a_k^\dagger a_k dk - \frac{\sqrt{\alpha}}{(2\pi)^{3/2}} \int_{\mathbb{R}^3} \left[ a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x} \right] \frac{dk}{|k|}, \tag{5.0.1}$$

where $\mathbf{p} = -i\nabla_x$ is the electron momentum operator, $\alpha > 0$ is the coupling parameter for the electron-phonon interaction and the external electric potential $V(x) \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ is nonnegative and vanishes at infinity. We motivate our results by discussing a polaron localized in a general potential $V(x)$ as above, but we shall work with a specific *radial* Mexican hat-type potential that we denote as $V_R(x)$ with $R > 2$, where $V_R(x) \in C_c^\infty(\mathbb{R}^3)$, $0 \leq V_R(x) \leq 1$ and

$$V_R(x) = \begin{cases} 0 & \text{when} \quad |x| \leq 1 \\ 1 & \text{when} \quad 2 \leq |x| \leq R \\ 0 & \text{when} \quad |x| \geq R+1 \end{cases} . \tag{5.0.2}$$

The Hamiltonian $H_\alpha^V$ is an operator on the Hilbert space $\mathcal{H} := L^2(\mathbb{R}^3) \otimes \mathcal{F}$, and $\mathcal{F} := \oplus_{n\geq 0} \otimes_s^n L^2(\mathbb{R}^3)$ is the (symmetric) phonon Fock space with scalar creation and annihlation operators $a_k^\dagger$ and $a_k$ satisfying the canonical commutation relation $[a_k, a_{k'}^\dagger] = \delta(k - k')$; we let $x \in \mathbb{R}^3$ denote the electronic coordinate and $k \in \mathbb{R}^3$ denote the phonon modes. The *ground-state energy* of the model is

$$E^V(\alpha) = \inf\left\{\left\langle \Psi,\ H_\alpha^V \Psi\right\rangle \mid \Psi \in L^2(\mathbb{R}^3) \otimes \mathcal{F} \text{ and } \|\Psi\| = 1\right\}, \tag{5.0.3}$$

and a normalized function in $L^2(\mathbb{R}^3) \otimes \mathcal{F}$ that achieves the infimum in (5.0.3) is called a *ground-state wave function.*

Using the now-standard techniques developed by F. Hiroshima [**Ha2000**] and M. Griesemer, E.H. Lieb and M. Loss [**GLL2001**] to study the analogous Pauli-Fierz model in quantum electrodynamics, it can be argued that, under physically natural conditions on the external potential, the Fröhlich Hamiltonian $H_\alpha^V$ has a unique ground state for all values of the coupling paramater $\alpha > 0$. Because it is straightforward to adapt the arguments in [**Ha2000**] and [**GLL2001**] to the Fröhlich Hamiltonian and because the arguments are rather long, we do not provide a proof of the existence and uniqueness of a ground state here. We describe the main ideas below:

Proposition 25. *Fix $\alpha > 0$. If the Schrödinger operator $\mathbf{p}^2 - \alpha^2 V(\alpha x)$ has a negative energy bound state in $L^2(\mathbb{R}^3)$, i.e., there is an eigenfunction $\zeta \in L^2(\mathbb{R}^3)$ and $\eta > 0$ so that*

$$\left(\mathbf{p}^2 - \alpha^2 V(\alpha x)\right)\zeta(x) = -\eta\zeta(x), \tag{5.0.4}$$

*then there exists a normalized function $\Psi_\alpha^V$ in $L^2(\mathbb{R}^3) \otimes \mathcal{F}$ satisfying*

$$H_\alpha^V \Psi_\alpha^V = E^V(\alpha)\, \Psi_\alpha^V.$$

The existence of a negative energy bound state of the operator $\mathbf{p}^2 - \alpha^2 V(\alpha x)$ can be used to show that the Fröhlich Hamiltonian $H_\alpha^V$ satisfies the binding condition (cf. Theorem 3.1 in [**GLL2001**])

$$E^V(\alpha) < E^{V\equiv 0}(\alpha). \tag{5.0.5}$$

With the Rellich-Kondrashov theorem and the binding inequality in (5.0.5), the above proposition can be established along the lines of the argument provided in [**GLL2001**]. In order to see that the ground state is unique, we use the well-known Schrödinger representation of the phonon Fock space $\mathcal{F}$, which is naturally identified with the $L^2$ space over a probability measure space $(\mathcal{Q}, \mu)$ (see p. 185 in [**Sp2004**]). We denote the unitary operator

$$\vartheta :\ L^2\left(\mathbb{R}^3\right) \otimes \mathcal{F} \mapsto L^2\left(\mathbb{R}^3 \otimes \mathcal{Q},\ dx \times d\mu\right). \tag{5.0.6}$$

The identification in (5.0.6) of $\mathcal{F}$ with an $L^2$ space opens up the possibility of establishing the uniqueness of the ground state via the classical route of positiviity improvement: on a

$\sigma-$finite measure space $(\chi, \nu)$, a bounded operator $B$ on $L^2(\chi, \nu)$ is positivity improving if $\langle f_1, B\, f_2\rangle_{L^2(\chi,\nu)} > 0$ for all positive $f_1$ and $f_2$ in $L^2(\chi, \nu)$ (and a function $f \in L^2(\chi, \nu)$ is positive if $f \geq 0$ a.e. and $f \neq 0$ a.e.). Armed with the Schrödinger representation and the notion of positivity improvement defined above, uniqueness can be shown along the lines of Hiroshima's argument in [**Ha2000**]:

PROPOSITION 26. *Fix $\alpha > 0$, and let the external potential $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ satisfy the conditions of Proposition 1 above. Writing $V = V_+ - V_-$, suppose $\alpha^2 V_+(\alpha x)$ is relatively form bounded with respect to the operator $\mathbf{p}^2$ with form bound strictly less than one; that is, for some $0 < a < 1$ there exists $c_a > 0$ such that for all $\xi \in H^1(\mathbb{R}^3)$,*

$$\alpha^2 \int_{\mathbb{R}^3} V_+(\alpha x)\, |\xi(x)|^2\, dx \leq a \|\nabla \xi\|_2^2 + c_a \|\xi\|_2^2. \tag{5.0.7}$$

*Then the ground-state wave function $\Psi_\alpha^V$ of the Fröhlich Hamiltonian $H_\alpha^V$ is unique.*

Let $\vartheta$ be the unitary operator as given in (5.0.6). When the external potential $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ satisfies the condition in (5.0.7), it is possible to show using the functional integral formula for the heat kernel that the operator $\vartheta e^{-tH_\alpha^V}\vartheta^{-1}$, $t > 0$ is positivity improving [**Ha2000**]. It then follows that the ground state of $\vartheta H_\alpha^V \vartheta^{-1}$ is unique (see p.191 in [**Sp2004**]). Since $\vartheta$ is unitary, the ground state of $H_\alpha^V$ is therefore also unique.

When the Hamiltonian $H_\alpha^V$ has a ground state $\Psi_\alpha^V$, we can integrate out the phonon coordinates and consider the *ground-state electron density*, $\|\Psi_\alpha^V\|_{\mathcal{F}}^2(x)$, which is a function of only the electron coordinate. If $V(x)$ is radial and the ground state $\Psi_\alpha^V$ is also unique, then $\Psi_\alpha^V$ is invariant after a rotation in *both* the electron and phonon coordinates. We state this precisely: Denoting $\hat{\mathbf{n}}$ to be a vector in $\mathbb{R}^3$, the field (phonon) angular momentum relative to the origin is given by the operator (see [**Sp2004**])

$$J_f = \int_{\mathbb{R}^3} dk\, (k \times i\nabla_k)\, a_k^\dagger a_k.$$

Let $\mathcal{R}_\theta \in SO(3)$ be a rotation by an angle $\theta$ about $\hat{\mathbf{n}}$. We say that $\Psi_\alpha^V$ is invariant under rotations when for any vector $\hat{\mathbf{n}} \in \mathbb{R}^3$ and all $\theta$,

$$\Psi_\alpha^V(x;\, k) = e^{-i\theta\hat{\mathbf{n}}\cdot J_f}\, \Psi_\alpha^V(\mathcal{R}_\theta x;\, k). \tag{5.0.8}$$

We can then deduce that the electron density $\|\Psi_\alpha^V\|_{\mathcal{F}}^2(x)$ is radial. We summarize this crucial observation: If the external potential $V(x)$ is radial and the Hamiltonian $H_\alpha^V$ has a unique ground-state wave function $\Psi_\alpha^V$, then its electron density $\|\Psi_\alpha^V\|_{\mathcal{F}}^2(x)$ is a radial function.

Unfortunately, the electron-phonon interaction term in the Hamiltonian makes it difficult to calculate essential quantities such as the effective mass and the ground-state energy, given in (5.0.3) above. By the 1950s, this mathematical difficulty motivated physicists to develop various techniques for approximating the effective mass and the ground state energy by exploiting the properties of the ground-state wave function. In 1951 Pekar developed a variational theory, built entirely on an Ansatz for the ground-state wave function: when the coupling parameter $\alpha$ is large, he guessed that the ground state has the product form

$$\Psi_\alpha = \psi_\alpha(x) \otimes \Phi_\alpha, \tag{5.0.9}$$

where $\psi_\alpha \in L^2(\mathbb{R}^3)$ is an electronic wave function, and $\Phi_\alpha \in \mathcal{F}$ is a coherent state depending only on the phonon coordinates:

$$\Phi_\alpha = \prod_k \exp\left(z_\alpha(k)a_k^\dagger - \overline{z_\alpha(k)}a_k\right)|0\rangle \tag{5.0.10}$$

with the vacuum $|0\rangle \in \mathcal{F}$ and the phonon displacements $z_\alpha(k) \in L^2(\mathbb{R}^3)$, which are determined variationally.

(Shortly thereafter, successful variational theories were also developed by Lee-Low-Pines (1953) and Feynman (1955) to address the weak and intermediate-coupling regimes using rather different Ansätze for the ground-state wave function.)

The optimization problem in (5.0.3) for the ground-state energy becomes considerably more tractable if we assume that the ground state has the product form in Pekar's Ansatz. Minimizing the quantity $\langle\Psi,\ H_\alpha^V\Psi\rangle$ over the more restrictive set of product wave functions in (5.0.9) and completing the square, Pekar deduced that

$$z_\alpha(k) = \frac{1}{\pi|k|}\sqrt{\frac{\alpha}{2}}\int_{\mathbb{R}^3} e^{-ik\cdot x}|\psi_\alpha|^2 dx, \tag{5.0.11}$$

which couples the coherent state to the electronic wave function in (5.0.9), and arrived at an *upper bound* for the ground-state energy:

$$\begin{aligned} E_\alpha^V &\le \inf\left\{\langle\Psi,\ H_\alpha^V\Psi\rangle \mid \|\Psi\| = 1 \text{ and } \Psi = \psi\otimes\Phi\right\} \\ &= \alpha^2 e(V). \end{aligned} \tag{5.0.12}$$

The quantity $e(V)$ in (5.0.12) can be calculated by minimizing the nonlinear *Pekar functional*:

$$e(V) = \inf_{\|\psi\|_2=1} \mathcal{E}_V(\psi) \tag{5.0.13}$$

$$= \inf_{\|\psi\|_2=1}\left\{\int_{\mathbb{R}^3}|\nabla\psi|^2 dx - \int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\psi(x)|^2\,|\psi(y)|^2}{|x-y|}dx\,dy - \int_{\mathbb{R}^3}V(x)|\psi(x)|^2 dx\right\}. \tag{5.0.14}$$

Furthermore, if the minimization problem problem in (5.0.13) admits a minimizer $\phi(x)$, then $\alpha^{3/2}\phi(\alpha x)$ is the electronic wave function in Pekar's product ground state from (5.0.9):

$$\Psi_\alpha = \alpha^{3/2}\phi(\alpha x)\prod_k \exp\left(z_\alpha(k)a_k^\dagger - \overline{z_\alpha(k)}a_k\right)|0\rangle, \tag{5.0.15}$$

where

$$z_\alpha(k) = \frac{1}{\pi|k|}\sqrt{\frac{\alpha}{2}}\int_{\mathbb{R}^3} e^{-ik\cdot x}|\alpha^{3/2}\phi(\alpha x)|^2 dx;$$

note that the electronic function becomes localized when the coupling parameter $\alpha > 0$ is large.

Though Pekar's result in (5.0.12) is only an upper bound, his Ansatz provides the convenience of eliminating all of the phonon coordinates from the calculation: the functional in (5.0.14) needs to be minimized just over a single electronic coordinate, a sharp contrast to the more demanding situation in (5.0.3).

The first detailed analysis of the nonlinear problem in (5.0.14) was given in 1977 by Lieb, who used symmetric decreasing rearrangement inequalities to show that a minimizer exists when $V = 0$. He also established that this minimizer is unique up to a translation by proving uniqueness of a radial solution for the corresponding Euler-Lagrange equation

$$\left\{-\triangle - 2\int_{\mathbb{R}^3} |\phi(y)|^2 |x-y|^{-1} dy\right\}\phi(x) = \phi(x),$$

known in the literature as the *Choquard-Pekar* or *Schrödinger-Newton equation*. For showing the existence of a minimizer with $V \neq 0$ in (5.0.14), Lieb's symmetrization argument applies only when $V(x)$ is a symmetric decreasing function. This motivated Lions to develop his famous Concentration Compactness Principle from 1984: for a general $V \geq 0$ that vanishes at infinity, he showed that the problem in (5.0.14) admits a minimizer. We provide a much simpler proof using the IMS Localization Formula.

Uniqueness of a minimizer when $V \neq 0$, however, remains an elusive open problem.

Despite giving rise to a rich variational theory that continues to be a source of interesting mathematical problems, Pekar's Produkt-Ansatz of the ground state in (5.0.9) lacks a rigorous justification: It is based entirely on his *feeling* that (we quote the amusing yet accurate, anthropomorphic description from [**LT1997**]) "...at large coupling the phonons cannot follow the rapidly moving electron (as they do at weak coupling) and so resign themselves to interacting with the "mean" electron density $\psi^2(\mathbf{x})$." This "mean-field" interaction is reflected in the phonon displacements, given in equation (5.0.11), for Pekar's coherent state.) Another unpleasant feature of Pekar's Ansatz, already alluded to in the second paragraph of the introduction, is it implies that the ground-state wave function of the translation-invariant (TI-) polaron is highly localized at large values of the coupling parameter. Indeed, his Ansatz for the TI-polaron only exacerbated the controversy generated by L.D. Landau's infamous two-page paper, first *suggesting* the phenomenon of self-localization in polaronic systems [Ld1933]. In fact, Pekar himself was one of the earliest critics of his Ansatz. In 1958, he attempted with V.M. Buimistrov to develop a translation-invariant theory for the TI-polaron by taking a "translational average" of his wave function in (5.0.15) In spite of all this controversy it is remarkable that Pekar's crude upper bound for the ground-state energy in (5.0.12)– derived after all from his unjustified Ansatz– becomes exact in the strong-coupling limit:

$$\lim_{\alpha\to\infty} \frac{E_\alpha^V}{\alpha^2} = e(V). \tag{5.0.16}$$

The convergence in (5.0.16) was argued formally ([**AGL1980**]) by J. Adamowski, B. Gerlach and H. Leschke in 1980 using the large deviation techniques (see [**DV1975**], [**DV1975-II**], [**DV1975-III**] and [**DV1976**]) developed by M.D. Donsker and S.R.S. Varadhan, who later provided a rigorous proof in [**DV1983**]. In 1997, Lieb and L.E. Thomas gave an alternate, pedestrian proof of the convergence in (5.0.16) using simple modifications of the Hamiltonian ([**LT1997**]), a philosophy that can be traced back to the inspiring work of Lieb and K. Yamazaki ([**LY1958**]).

In light of the convergence in (5.0.16) for the ground state energy, it is now only natural to investigate how well Pekar's theory describes the ground-state wave function (in the strong-coupling limit). Let $\|\Psi_\alpha^V\|_{\mathcal{F}}^2(x)$ denote the electron density of the ground state, and recall that a minimizer of the Pekar functional from (5.0.14) is the electronic wave function in his Produkt-Ansatz. Since the ground state energy in the strong-coupling limit can be obtained by minimizing the Pekar functional, shouldn't the electron density $\|\Psi_\alpha^V\|_{\mathcal{F}}^2$ also converge to a minimizer of the Pekar functional? If the minimizer of the functional is unique, then it is possible to prove such a convergence:

THEOREM 27. *Suppose the external potential $V(x)$ satisfies the conditions in (5.0.4) and let $\Psi_\alpha^V \in \mathcal{H}$ be a ground-state wave function of the Fröhlich Hamiltonian $H_\alpha^V$ in (5.0.1). If the minimization problem in (5.0.14) for the Pekar energy admits a unique minimizer $u_V$, then*

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi_\alpha^V\|_{\mathcal{F}}^2 \left(\frac{x}{\alpha}\right) W(x)\, dx = \int_{\mathbb{R}^3} |u_V(x)|^2\, W(x)\, dx \tag{5.0.17}$$

*for all $W \in L^{\frac{3}{2}}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.*

The essence of the proof lies in differentiating the (concave) map $\delta \mapsto e(V+\delta W)$ at $\delta = 0$, where

$$e(V+\delta W) = \inf_{\|\psi\|_2=1} \left\{ \mathcal{E}_V(\psi) - \delta \int_{\mathbb{R}^3} |\psi(x)|^2\, W(x)\, dx \right\},$$

for which we need uniqueness, as demonstrated in the above chapter.

However, it is not necessarily the case that the Pekar minimization problem admits a unique minimizer: consider, for example, the potential $V_R(x)$ given in (5.0.2) above. For each $\alpha > 0$ the Hamiltonian $H_\alpha^{V_R}$, $R > 2$ has a unique ground-state wave function. Since the potential $V_R(x) \geq 0$ is short-range, i.e. decays exponentially at infinity, it is known that for each $\alpha > 0$ the Schrödigner operator $\mathbf{p}^2 - \alpha^2 V_R(\alpha x)$ has a negative energy bound state in $L^2(\mathbb{R}^3)$ (see e.g. the introduction in [**BV2004**]). (To be precise: For the short-range potential $V_R(x)$ it can be seen that there exists *for all* $\alpha > 0$ some $\lambda_0 > 0$ such that for $\lambda > \lambda_0$ the operator $\mathbf{p}^2 - \lambda\alpha^2 V(\alpha x)$ has a negative energy bound state in $L^2(\mathbb{R}^3)$. But our proofs still hold true if for some $\lambda > \lambda_0$ the function $V_R(x)$ in (5.0.2) is replaced by $\lambda V_R(x)$, so we do not inconvenience ourselves any further with this innocuous technicality.) Furthermore, since $V_R(x) \geq 0$ and $V_R \in L^\infty(\mathbb{R}^3)$, the form bound in (5.0.7) follows trivially from Hölder's inequality. The potential $V_R$, $R > 2$ satisfies the conditions set forth in the above two propositions. Hence, for $R > 2$ there exists a unique ground-state wave function $\Psi_\alpha^{V_R}$. The uniqueness of the ground state together with the radiality of $V_R$ imply that the ground-state electron density $\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2(x)$ is radial. But now, we show that the minimizers of the Pekar functional are not radial.

THEOREM 28. *Let the Pekar minimization problem $e(V)$ be as defined in (5.0.14) above and let the Mexican hat-type potential $V_R$ be as given in (5.0.2). For $R$ large the Pekar minimization problem $e(V_R)$ admits only nonradial minimizers.*

So, the kind of convergence in (5.0.17) is not possible. Nevertheless it is possible to show that–under a uniqueness up to rotations assumption–the electronic density converges to a rotational average of the densities of the nonradial Pekar minimizers!

THEOREM 29. *let $\Psi_\alpha^{V_R} \in \mathcal{H}$ be the unique ground-state wave function of the Fröhlich Hamiltonian $H_\alpha^{V_R}$ in (5.0.1). If the minimization problem in (5.0.14) for the Pekar energy admits a minimizer $u_{V_R}$ that is unique up to a rotation, then, denoting $\gamma$ to be the Haar measure on $SO(3)$,*

$$\lim_{\alpha\to\infty} \frac{1}{\alpha^3} \int_{\mathbb{R}^3} \|\Psi_\alpha^V\|_{\mathcal{F}}^2 \left(\frac{x}{\alpha}\right) W(x)\, dx = \int_{\mathbb{R}^3} \left[\int_{SO(3)} |u_{V_R}(\mathcal{R}x)|^2\, d\gamma(\mathcal{R})\right] W(x)\, dx \tag{5.0.18}$$

*for all $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$.*

First, the non-radiality of the minimizes will be argued.

### 5.1. Nonradiality of the Pekar Minimizers

The existence of minimizers for the Pekar minimization problem will have to be argued. We prove this for general potential (satisfying a very natural binding condition). The proof forgoes the use of complicated machinery such as Lions' concentration compactness argument. Rather, we can argue compactness using a (very natural) binding condition and the IMS Localization Formula.

LEMMA 30. *Let $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ vanish at infinity, and let the energies $e(V)$ and $e(0)$ be as defined in (5.0.14) above. Suppose that $e(V) < e(0)$. If $\{\varphi_n\}_{n=1}^\infty$ is a minimizing sequence for the energy $e(V)$, then there exists some subsequence $\{\varphi_{n_k}\}_{k=1}^\infty$ satisfying the following property: for any given $\epsilon > 0$, there is some $R > 0$ such that*

$$\|\varphi_{n_k}\|^2_{L^2(\{|x|<R\})} > 1 - \epsilon. \tag{5.1.1}$$

PROOF. We write $V = V_1 + V_2$, where $V_1 \in L^{3/2}(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$. First, we need to show that $e(V) > -\infty$.

**Step 1** (Energy is Bounded from Below). Let $u \in H^1(\mathbb{R}^3)$ and $\|u\|_2 = 1$. We recall the Sobolev inequality, $\|\nabla u\|_2^2 \geq S\|u\|_6^2$ with the best constant $S = 3\,(\pi/2)^{4/3}$. Moreover, since $V_1 \in L^{3/2}(\mathbb{R}^3)$, we know using the Dominated Convergence Theorem that there exists some $\lambda > 0$ where $\|(V-\lambda)_+\|_{3/2} < S/4$. Writing $|x|^{-1} = h_{1;\beta}(x) + h_{2;\beta}(x)$, where

$$h_{1;\beta}(x) = |x|^{-1}\chi^{(x)}_{\{|x|\leq\beta\}} \quad \text{and} \quad h_{2;\beta}(x) = |x|^{-1}\chi^{(x)}_{\{|x|>\beta\}},$$

we see using the Sobolev and Young's inequalities that

$$\begin{aligned}
\mathcal{E}_V(u) &\geq \|\nabla u\|_2^2 - \|h_{1;\beta}\|_{\frac{3}{2}}\|u\|_6^2 - \beta^{-1} - \|(V_1-\lambda)_+\|_{\frac{3}{2}}\|u\|_6^2 - \|V_2\|_\infty - \lambda \\
&\geq \|\nabla u\|_2^2 - S^{-1}\|h_{1;\beta}\|_{\frac{3}{2}}\|\nabla u\|_2^2 - \beta^{-1} - S^{-1}\|\left(V_1-\lambda\right)_+\|_{\frac{3}{2}}\|\nabla u\|_2^2 - \|V_2\|_\infty - \lambda \\
&= \|\nabla u\|_2^2\left(1 - S^{-1}\left(\|h_{1;\beta}\|_{\frac{3}{2}} + \|(V_1-\lambda)_+\|_{\frac{3}{2}}\right)\right) - \left(\beta^{-1} + \|V_2\|_\infty + \lambda\right).
\end{aligned}$$

Furthermore, $\|h_{1;\beta}\|_{3/2} = (4\pi)^{2/3}\beta^{1/3}$, and we choose $\beta$ small so that $\|h_{1;\beta}\|_{3/2} < S/4$. Then for *any* $u \in H^1(\mathbb{R}^3)$ such that $\|u\|_2 = 1$, we have

$$\begin{aligned}
\mathcal{E}_V(u) &\geq \frac{1}{2}\|\nabla u\|_2^2 - \left(\beta^{-1} + \|V_2\|_\infty + \lambda\right) \\
&\geq -\left(\beta^{-1} + \|V_2\|_\infty + \lambda\right) > -\infty.
\end{aligned} \tag{5.1.2}$$

Hence,

$$e(V) = \inf_{\|u\|_2=1} \mathcal{E}_V(u) > -\infty.$$

**Step 2** (Extracting a Weak Limit). Since $e(V) > -\infty$ and $\{\varphi_n\}_{n=1}^\infty$, $\|\varphi_n\|_2 = 1$ is a minimizing sequence for the energy $e(V)$, it is clear that for large $n$

$$\mathcal{E}_V(\varphi_n) < e(V) + 1. \tag{5.1.3}$$

From the inequalities in (5.1.2) and (5.1.3) above, we deduce that for $n$ large,

$$\|\nabla\varphi_n\|_2^2 \leq 2\left(e(V) + 1 + \beta^{-1} + \|V_2\|_\infty + \lambda\right). \tag{5.1.4}$$

Since $e(V) < \infty$, we observe from (5.1.4) that the minimizing sequence $\{\varphi_n\}_{n=1}^{\infty}, \|\varphi_n\|_2 = 1$ is uniformly bounded in $H^1(\mathbb{R}^3)$. For all $n$,

$$\|\nabla\varphi_n\|_{H^1} < C. \tag{5.1.5}$$

Then there exists some subsequence $\{\varphi_{n_k}\}_{k=1}^{\infty}$ and some $\varphi \in H^1(\mathbb{R}^3)$ such that (Theorem 2.18 in [**LL2001**])

$$\varphi_{n_k} \rightharpoonup \varphi \ \text{ in } \ H^1\left(\mathbb{R}^3\right). \tag{5.1.6}$$

The goal in the rest of the proof is to show that the weakly convergent subsequence satisfies the condition in (5.1.1).

It now follows from the Sobolev inequality and the uniform bound in (5.1.5) that $\|\varphi_{n_k}\|_6 < C$ for all $k$. We then observe from the weak lower semicontinuity of the $L^p$-norm that $\varphi \in L^6(\mathbb{R}^3)$. Since $\|\varphi_{n_k}\|_2 = 1$ and $\|\varphi\|_2 \leq 1$, we can conclude that for all $k$,

$$\|\varphi_{n_k}\|_p < C \ \text{ and } \ \varphi \in L^p\left(\mathbb{R}^3\right) \ \text{ for } \ 2 \leq p \leq 6. \tag{5.1.7}$$

**Step 3** (Rellich-Kondrashov Theorem). First we note that for any given $\epsilon > 0$, there exists some $R > 0$ such that

$$\frac{1}{R} < \epsilon, \tag{5.1.8}$$

$$|V(x)| < \epsilon \ \text{ for all } \ |x| > \frac{R}{2}, \tag{5.1.9}$$

and

$$\|\varphi\|^2_{L^{12/5}(\{|x|>R/2\})} < \frac{\epsilon}{4}. \tag{5.1.10}$$

Above, (5.1.9) follows from the fact that the external potential $V(x)$ vanishes at infinity, and (5.1.10) follows from our observation in (5.1.7).

Since the (minimizing) subsequence $\{\varphi_{n_k}\}_{k=1}^{\infty}$ converges weakly in $H^1(\mathbb{R}^3)$ to $\varphi$, we observe from the Rellich-Kondrashov Theorem (Theorem 8.6 in [**LL2001**]) that for any given $\epsilon > 0$ and $R > 0$ satisfying the conditions in (5.1.8), (5.1.9) and (5.1.10) above, there exists some $N > 0$ such that for all $n_k > N$

$$\|\varphi_{n_k} - \varphi\|_{L^{12/5}(\{\frac{R}{2} \leq |x| < 3R\})} < \frac{\sqrt{\epsilon}}{2}, \tag{5.1.11}$$

and for all $n_k > N$ (since $\{\varphi_{n_k}\}_{k=1}^{\infty}$ is minimizing for $e(V)$)

$$\mathcal{E}_V\left(\varphi_{n_k}\right) < e(V) + \epsilon. \tag{5.1.12}$$

It is now clear from (5.1.10) and (5.1.11) that for all $n_k > N$

$$\|\varphi_{n_k}\|^2_{L^{12/5}\left(\left\{\frac{R}{2} \leq |x| < 3R\right\}\right)} < \epsilon. \tag{5.1.13}$$

The bound in (5.1.13) above will be useful in the next step, where we use the well-known IMS Localization technique:

**Step 4** (IMS Localization). There exist real-valued functions $\chi, \tilde{\chi} \in C_c^{\infty}(\mathbb{R}^3)$ such that $0 \leq \chi(x) \leq 1$ and $0 \leq \tilde{\chi}(x) \leq 1$, where

$$\chi(x) = \begin{cases} 1 & \text{when } |x| \leq \frac{1}{2} \\ 0 & \text{when } |x| > 1 \end{cases} \qquad \text{and} \qquad \tilde{\chi}(x) = \begin{cases} 0 & \text{when } |x| \leq \frac{1}{2} \\ 1 & \text{when } |x| > 1 \end{cases} \tag{5.1.14}$$

and

$$\chi^2(x) + \tilde{\chi}^2(x) = 1 \quad \text{for all } x \in \mathbb{R}^3. \tag{5.1.15}$$

For a given $\epsilon > 0$, let $R > 0$ satisfy the properties in (5.1.8), (5.1.9) and (5.1.10) above. In the rest of the proof, we shall consider the scaled functions $\chi_{_R}(x) = \chi\left(\frac{x}{R}\right)$ and $\tilde{\chi}_{_R}(x) = \tilde{\chi}\left(\frac{x}{R}\right)$. Since $\|\varphi_{n_k}\|_2 = 1$, we observe that $\|\chi_{_R}\varphi_{n_k}\|_2 \le 1$ and $\|\tilde{\chi}_{_R}\varphi_{n_k}\|_2 \le 1$ for all $k$ and (from (5.1.15) above) that

$$\|\chi_{_R}\varphi_{n_k}\|_2^2 + \|\tilde{\chi}_{_R}\varphi_{n_k}\|_2^2 = 1.$$

Furthermore, we can see from an elementary computation that for any $\varphi \in H^1(\mathbb{R}^3)$,

$$\int_{\mathbb{R}^3} |\nabla\varphi|^2\,dx = \int_{\mathbb{R}^3} |\nabla(\chi_{_R}\varphi)|^2\,dx + \int_{\mathbb{R}^3} |\nabla(\tilde{\chi}_{_R}\varphi)|^2\,dx - \int_{\mathbb{R}^3} |\varphi|^2\left(|\nabla\chi_{_R}|^2 + |\nabla\tilde{\chi}_{_R}|^2\right)dx,$$

$$\begin{aligned}
&\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|}\,dx\,dy \\
&= \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|(\chi_{_R}\varphi)(x)|^2\,|(\chi_{_R}\varphi)(y)|^2}{|x-y|}\,dx\,dy + \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|(\tilde{\chi}_{_R}\varphi)(x)|^2\,|(\tilde{\chi}_{_R}\varphi)(y)|^2}{|x-y|}\,dx\,dy \\
&\qquad + 2\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|(\chi_{_R}\varphi)(x)|^2\,|(\tilde{\chi}_{_R}\varphi)(y)|^2}{|x-y|}\,dx\,dy,
\end{aligned}$$

and

$$\int_{\mathbb{R}^3} V(x)|\varphi(x)|^2dx = \int_{\mathbb{R}^3} V(x)\,|(\chi_{_R}\varphi)(x)|^2\,dx + \int_{\mathbb{R}^3} V(x)\,|(\tilde{\chi}_{_R}\varphi)(x)|^2\,dx.$$

With our (minimizing) subsequence $\{\varphi_{n_k}\}_{k=1}^{\infty}$, $\|\varphi_{n_k}\|_2 = 1$ above, we then calculate

$$\begin{aligned}
\mathcal{E}_V(\varphi_{n_k}) = \mathcal{E}_V(\chi_{_R}\varphi_{n_k}) + \mathcal{E}_V(\tilde{\chi}_{_R}\varphi_{n_k}) - 2\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|(\chi_{_R}\varphi_{n_k})(x)\right|^2\left|(\tilde{\chi}_{_R}\varphi_{n_k})(y)\right|^2}{|x-y|}\,dx\,dy \\
- \int_{\mathbb{R}^3} |\varphi_{n_k}|^2\left(|\nabla\chi_{_R}|^2 + |\nabla\tilde{\chi}_{_R}|^2\right)dx.
\end{aligned} \tag{5.1.16}$$

For any $\varphi \in H^1(\mathbb{R}^3)$ such that $0 < \|\varphi\|_2 \le 1$, since $\|\varphi\|_2^4 \le \|\varphi\|_2^2$, we have

$$\begin{aligned}
e(V) &\le \mathcal{E}_V\left(\frac{\varphi}{\|\varphi\|_2}\right) \\
&= \frac{1}{\|\varphi\|_2^2}\int_{\mathbb{R}^3} |\nabla\varphi|^2dx - \frac{1}{\|\varphi\|_2^4}\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|}\,dx\,dy - \frac{1}{\|\varphi\|_2^2}\int_{\mathbb{R}^3} V(x)|\varphi(x)|^2dx \\
&\le \frac{1}{\|\varphi\|_2^2}\int_{\mathbb{R}^3} |\nabla\varphi|^2dx - \frac{1}{\|\varphi\|_2^2}\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|}\,dx\,dy - \frac{1}{\|\varphi\|_2^2}\int_{\mathbb{R}^3} V(x)|\varphi(x)|^2dx \\
&= \frac{1}{\|\varphi\|_2^2}\mathcal{E}_V(\varphi).
\end{aligned}$$

The above reasoning also holds true when $V = 0$. Then for $\varphi \in H^1(\mathbb{R}^3)$, we have

$$\mathcal{E}_V(\varphi) \ge e(V)\|\varphi\|_2^2 \quad \text{and} \quad \mathcal{E}_0(\varphi) \ge e(0)\|\varphi\|_2^2 \quad \text{when} \quad \|\varphi\|_2 \le 1. \tag{5.1.17}$$

For our (minimizing) subsequence $\{\varphi_{n_k}\}_{k=1}^{\infty}$ where $\|\varphi_{n_k}\|_2 = 1$, since $\|\chi_{_R}\varphi_{n_k}\|_2 \le 1$ and $\|\tilde{\chi}_{_R}\varphi_{n_k}\|_2 \le 1$ for all $k$, we deduce from our calculation in (5.1.16) above and from (5.1.17) that

$$\mathcal{E}_V\left(\varphi_{n_k}\right) \geq e(V)\|\chi_R\varphi_{n_k}\|_2^2 + e(0)\|\tilde{\chi}_R\varphi_{n_k}\|_2^2 - \int_{\mathbb{R}^3} V(x)\left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(x)\right|^2 dx$$

$$- \int_{\mathbb{R}^3} \left|\varphi_{n_k}\right|^2 \left(|\nabla\chi_R|^2 + |\nabla\tilde{\chi}_R|^2\right) dx - 2\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy.$$

Furthermore, $\|\tilde{\chi}_R\varphi_{n_k}\|_2^2 = 1 - \|\chi_R\varphi_{n_k}\|_2^2$, and

$$\mathcal{E}_V\left(\varphi_{n_k}\right) \geq \left(e(V) - e(0)\right)\|\chi_R\varphi_{n_k}\|_2^2 + e(0) - \int_{\mathbb{R}^3} V(x)\left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(x)\right|^2 dx$$

$$- \int_{\mathbb{R}^3} \left|\varphi_{n_k}\right|^2 \left(|\nabla\chi_R|^2 + |\nabla\tilde{\chi}_R|^2\right) dx - 2\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy.$$

The task now is to show that the last three terms on the right-hand side of the inequality above are small:

**Step 5** (Last Three Terms are Small). Let $\epsilon > 0$ and $R > 0$ be as above. For the first term, since $\|\tilde{\chi}_R\varphi_{n_k}\|_2^2 \leq 1$ and $\tilde{\chi}_R(x) = 0$ for $|x| \leq R/2$, it follows from Hölder's inequality and (5.1.9) that for all $k$,

$$\int_{\mathbb{R}^3} V(x)\left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(x)\right|^2 dx < \epsilon. \tag{5.1.18}$$

Since $\chi, \tilde{\chi} \in C_c^\infty(\mathbb{R}^3)$, we know that $|\nabla\chi(x)|^2 + |\nabla\tilde{\chi}(x)|^2 < C$ for all $x \in \mathbb{R}^3$. For the second term, it then follows from Hölder's inequality and (5.1.8) that for all $k$,

$$\int_{\mathbb{R}^3} \left|\varphi_{n_k}\right|^2 \left(|\nabla\chi_R|^2 + |\nabla\tilde{\chi}_R|^2\right) dx < \frac{C}{R^2} < C\epsilon^2. \tag{5.1.19}$$

Finally, since $\tilde{\chi}_R(x) = 0$ for $|x| \leq R/2$ and $\chi_R(x) = 0$ when $|x| > R$, we can decompose the last term

$$\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy$$

$$= \int\int_{\mathbb{R}^3\times\left\{\frac{R}{2}\leq|y|\leq 3R\right\}} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy$$

$$+ \int\int_{\{|x|\leq R\}\times\{|y|>3R\}} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy.$$

With the second term in the above decomposition, we observe using (5.1.8) that for all $k$,

$$\int\int_{\{|x|\leq R\}\times\{|y|>3R\}} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2 \left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|} dx\, dy \leq \frac{1}{2R}\|\chi_R\varphi_{n_k}\|_2^2 \|\tilde{\chi}_R\varphi_{n_k}\|_2^2 < \frac{\epsilon}{2}.$$

Now we deal with the first term in the above decomposition. We recall our observation in (5.1.7) that for all $k$, $\|\varphi_{n_k}\|_{12/5}^2 < C$. Furthermore, as we already noted in (5.1.13),

$$\|\varphi_{n_k}\|^2_{L^{12/5}\left(\left\{\frac{R}{2}\le|x|<3R\right\}\right)} < \epsilon \quad \text{when} \quad n_k > N.$$

It then follows from the Hardy-Littlewood-Sobolev inequality that for $n_k > N$,

$$\begin{aligned}
&\int\int_{\mathbb{R}^3\times\left\{\frac{R}{2}\le|y|\le 3R\right\}} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2\left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|}dx\,dy \\
&\le C_{\mathrm{HLS}}\|\chi_R\varphi_{n_k}\|_{12/5}^2\|\tilde{\chi}_R\varphi_{n_k}\|^2_{L^{12/5}\left(\left\{\frac{R}{2}\le|x|\le3R\right\}\right)} \\
&< C\|\tilde{\chi}_R\varphi_{n_k}\|^2_{L^{12/5}\left(\left\{\frac{R}{2}\le|x|\le3R\right\}\right)} < C\epsilon.
\end{aligned}$$

We therefore conclude that for $n_k > N$,

$$\int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\left(\chi_R\varphi_{n_k}\right)(x)\right|^2\left|\left(\tilde{\chi}_R\varphi_{n_k}\right)(y)\right|^2}{|x-y|}dx\,dy \le \left(C+\frac{1}{2}\right)\epsilon. \tag{5.1.20}$$

**Step 6** (Conclusion). We recall from (5.1.12) that

$$\mathcal{E}_V\left(\varphi_{n_k}\right) < e(V)+\epsilon \quad \text{when} \quad n_k > N.$$

It follows from the last inequality in Step 4 and from (5.1.18), (5.1.19) and (5.1.20) above that for $n_k > N$,

$$e(V)+\epsilon > \mathcal{E}_V\left(\varphi_{n_k}\right) \ge \left(e(V)-e(0)\right)\|\chi_R\varphi_{n_k}\|_2^2 + e(0) - \left(\epsilon + C\epsilon^2 + \left(C+\frac{1}{2}\right)\epsilon\right).$$

Since, by assumption, $e(V) < e(0)$, we have for $n_k > N$

$$\|\chi_R\varphi_{n_k}\|_2^2 \ge 1 - \left(\frac{2\epsilon + C\epsilon^2 + \left(C+\frac{1}{2}\right)\epsilon}{e(0)-e(V)}\right). \tag{5.1.21}$$

Above $\epsilon > 0$ is arbitrary, and the claim in (5.1.1) follows.

□

Theorem 31. *Let $V \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ vanish at infinity, and let the energies $e(V)$ and $e(0)$ be as defined in (5.0.14) above. If $e(V) < e(0)$, then the minimization problem in (5.0.14) for the energy $e(V)$ admits a minimizer. Furthermore, any sequence $\{\varphi_n\}_{n=1}^\infty$, $\|\varphi_n\|_2 = 1$ satisfying*

$$\lim_{n\to\infty}\mathcal{E}_V\left(\varphi_n\right) = e(V)$$

*has a subsequence converging strongly in $H^1\left(\mathbb{R}^3\right)$ to some $\varphi \in H^1\left(\mathbb{R}^3\right)$ that is a minimizer for the energy $e(V)$, i.e., $\|\varphi\|_2 = 1$ and $\mathcal{E}_V\left(\varphi\right) = e(V)$.*

Proof. We proceed in the usual way by extracting a weakly convergent subsequence:

**Step 1** (Extracting a Weak Limit). In the proof of the above lemma it has been established in (5.1.5) that a minimizing sequence $\{\varphi_n\}_{n=1}^\infty$, $\|\varphi_n\|_2 = 1$ is uniformly bounded in $H^1\left(\mathbb{R}^3\right)$, i.e., $\|\varphi_n\|_{H^1(\mathbb{R}^3)} < C$. Then there exists a subsequence $\{\varphi_{n_k}\}_{k=1}^\infty$ and some

$\varphi \in H^1(\mathbb{R}^3)$ such that

$$\varphi_{n_k} \rightharpoonup \varphi \quad \text{in} \quad H^1\left(\mathbb{R}^3\right).$$

In the above lemma we have shown that the weakly convergent subsequence $\{\varphi_{n_k}\}_{k=1}^{\infty}$ satisfies the property given in (5.1.1) above. Moreover,

$$\liminf_{k\to\infty} \|\nabla\varphi_{n_k}\|_2 \geq \|\nabla\varphi\|_2, \tag{5.1.22}$$

and

$$1 = \liminf_{k\to\infty} \|\varphi_{n_k}\|_2 \geq \|\varphi\|_2, \tag{5.1.23}$$

and, as we already observed in (5.1.7) using the Sobolev inequality, we have for all $k$,

$$\|\varphi_{n_k}\|_p < C \quad \text{and} \quad \varphi \in L^p\left(\mathbb{R}^3\right) \quad \text{for} \quad 2 \leq p \leq 6. \tag{5.1.24}$$

An important consequence of the above Lemma is that $\|\varphi\|_2 = 1$:

**Step 2** (Weak Limit has Norm One). Since $\varphi_{n_k} \rightharpoonup \varphi$ in $H^1(\mathbb{R}^3)$, we observe from the Rellich-Kondrashov Theorem (Theorem 8.6 in [LL2001]) that for all $R > 0$,

$$\|\varphi_{n_k} - \varphi\|_{L^p(\{|x|\leq R\})} \longrightarrow 0, \quad p < 6. \tag{5.1.25}$$

It now follows from the above Lemma that

$$\|\varphi_{n_k} - \varphi\|_2 \longrightarrow 0 \quad \text{and} \quad \|\varphi\|_2 = 1. \tag{5.1.26}$$

We will show that $\varphi$ is a minimizer for the energy $e(V)$ by arguing the weak lower semicontinuity of the functional $\mathcal{E}_V$:

$$\liminf_{n\to\infty} \mathcal{E}_V(\varphi_n) \geq \mathcal{E}_V(\varphi), \tag{5.1.27}$$

and we recall that

$$\mathcal{E}_V(\phi) = \int_{\mathbb{R}^3} |\nabla\phi|^2 dx - \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\phi(x)|^2\,|\phi(y)|^2}{|x-y|} dx\,dy - \int_{\mathbb{R}^3} V(x)|\phi(x)|^2 dx.$$

**Step 3** (Weak Continuity of the Potential Energy). We begin by arguing that

$$\int_{\mathbb{R}^3} V(x)|\varphi_{n_k}(x)|^2 dx \longrightarrow \int_{\mathbb{R}^3} V(x)|\varphi(x)|^2 dx. \tag{5.1.28}$$

Writing $V = V_1 + V_2$, where $V_1 \in L^{3/2}(\mathbb{R}^3)$ and $V_2 \in L^\infty(\mathbb{R}^3)$ we have

$$\left|\int_{\mathbb{R}^3} V(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi|^2\right) dx\right|$$

$$\leq \left|\int_{\mathbb{R}^3} V_1(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx\right| + \left|\int_{\mathbb{R}^3} V_2(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx\right|. \tag{5.1.29}$$

For $0 < \delta < 1$, we introduce the truncated functions

$$V_1^\delta(x) = \begin{cases} V_1(x) & \text{when} \quad |V_1(x)| \leq \frac{1}{\delta} \\ 0 & \text{when} \quad |V_1(x)| > \frac{1}{\delta} \end{cases}.$$

Let $\epsilon > 0$. Using the Dominated Convergence Theorem, we know there exists some $0 < \delta < 1$ such that

$$\|V_1^\delta - V_1\|_{\frac{3}{2}} < \epsilon. \tag{5.1.30}$$

Furthermore, for $\epsilon > 0$, there exist $R > 0$ and $N > 0$ such that

$$\|V_1\|_{L^{3/2}(\{|x|>R\})} < \epsilon, \tag{5.1.31}$$

$$\|\varphi_{n_k}\|^2_{L^2(\{|x|\le R\})} > 1-\epsilon \ \text{ for } \ n_k > N, \tag{5.1.32}$$

$$\|\varphi\|^2_{L^2(\{|x|\le R\})} > 1-\epsilon, \tag{5.1.33}$$

$$\left\|\varphi_{n_k} - \varphi\right\|_{L^{12/5}(\{|x|\le R\})} < \epsilon \ \text{ for } \ n_k > N, \tag{5.1.34}$$

and with $0 < \delta < 1$ satisfying the condition in (5.1.30) above,

$$\left\|\varphi_{n_k} - \varphi\right\|_{L^2(\{|x|\le R\})} < \epsilon\delta \ \text{ for } \ n_k > N. \tag{5.1.35}$$

The condition in (5.1.32) is given by the above Lemma, (5.1.33) follows from (5.1.26), and (5.1.34) and (5.1.35) follow from our observation in (5.1.25).

We consider the first term in (5.1.29). We write

$$\int_{\mathbb{R}^3} V_1(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx$$

$$= \int_{\{|x|\le R\}} V_1(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx + \int_{\{|x|>R\}} V_1(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx. \tag{5.1.36}$$

For a given $\epsilon > 0$, let $0 < \delta < 1$, $R > 0$ and $N > 0$ satisfy the above properties. We now deal with the term on the left in (5.1.36). From (5.1.24), (5.1.30), (5.1.35) and Hölder's inequality, we observe that for all $n_k > N$,

$$\begin{aligned}
&\left|\int_{\{|x|\le R\}} V_1(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx\right| \\
&= \left|\int_{\{|x|\le R\}} \left[V_1(x) - V_1^\delta(x)\right]\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx\right| \\
&\qquad\qquad + \left|\int_{\{|x|>R\}} V_1^\delta(x)\left(|\varphi_{n_k}(x)|^2 - |\varphi(x)|^2\right) dx\right| \\
&\le \left\|V_1 - V_1^\delta\right\|_{\frac{3}{2}} \left\|\left|\varphi_{n_k}\right|^2 - |\varphi|^2\right\|_3 + \left\|V_1^\delta\right\|_\infty \left\|\left|\varphi_{n_k}\right|^2 - |\varphi|^2\right\|_{L^1(\{|x|\le R\})} \\
&< \epsilon\left(\left\|\varphi_{n_k}\right\|_6^2 + \|\varphi\|_6^2\right) + \frac{2}{\delta}\left\|\varphi_{n_k} - \varphi\right\|_{L^2(\{|x|\le R\})} < C\epsilon + 2\epsilon. \qquad (5.1.37)
\end{aligned}$$

We also see from the bound in (5.1.31) that for all $n_k > N$,

$$\left|\int_{\{|x|>R\}} V_1(x)\left(\left|\varphi_{n_k}\right|^2 - |\varphi|^2\right) dx\right| \le \|V_1\|_{L^{\frac{3}{2}}(\{|x|>R\})}\left(\left\|\varphi_{n_k}\right\|_6^2 + \|\varphi\|_6^2\right) < C\epsilon. \tag{5.1.38}$$

We now consider the second term in (5.1.29). We observe from (5.1.32), (5.1.35) and Hölder's inequality that for all $n_k > N$,

$$
\begin{aligned}
&\left|\int_{\mathbb{R}^3} V_2(x)\left(\left|\varphi_{n_k}\right|^2-|\varphi|^2\right)dx\right| \\
&\quad\leq 2\left\|V_2\right\|_\infty\left\|\varphi_{n_k}-\varphi\right\|_2
\end{aligned}
$$

$$
\leq 2\left\|V_2\right\|_\infty\left(\left\|\varphi_{n_k}-\varphi\right\|_{L^2(\{|x|\leq R\})}+\left\|\varphi_{n_k}\right\|_{L^2(\{|x|>R\})}+\|\varphi\|_{L^2(\{|x|>R\})}\right)\leq 6\epsilon\left\|V_2\right\|_\infty. \tag{5.1.39}
$$

Since $\epsilon$ is arbitrary, the weak continuity in (5.1.28) of the potential energy follows from (5.1.37), (5.1.38) and (5.1.39).

**Step 4** (Weak Continuity of the Coulomb Energy). It now remains to argue the weak continuity of the Coulomb energy:

$$
\left|\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\left|\varphi_{n_k(x)}\right|^2\left|\varphi_{n_k}(y)\right|^2}{|x-y|}dx\,dy-\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|}dx\,dy\right|\longrightarrow 0 \tag{5.1.40}
$$

For any given $\epsilon>0$, let $R>0$ and $N>0$ satisfy the aforementioned properties from (5.1.31) to (5.1.35). It follows from the positivity of the Coulomb energy (Theorem 9.8 in [**LL2001**]) and the Hardy-Littlewood-Sobolev inequality that

$$
\begin{aligned}
&\left|\left(\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\left|\varphi_{n_k(x)}\right|^2\left|\varphi_{n_k}(y)\right|^2}{|x-y|}dx\,dy\right)^{\frac{1}{2}}-\left(\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{|\varphi(x)|^2\,|\varphi(y)|^2}{|x-y|}dx\,dy\right)^{\frac{1}{2}}\right| \\
&\quad\leq\left|\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\left(\left|\varphi_{n_k}(x)\right|^2-|\varphi(x)|^2\right)\left(\left|\varphi_{n_k}(y)\right|^2-|\varphi(y)|^2\right)}{|x-y|}dx\,dy\right|^{\frac{1}{2}}
\end{aligned}
$$

$$
\leq C_{\mathrm{HLS}}^{1/2}\left(\left\|\left|\varphi_{n_k}\right|^2-|\varphi|^2\right\|_{L^{6/5}(\{|x|\leq R\})}+\left\|\left|\varphi_{n_k}\right|^2-|\varphi|^2\right\|_{L^{6/5}(\{|x|>R\})}\right). \tag{5.1.41}
$$

We recall the uniform bound in (5.1.24). From (5.1.34) and Hölder's inequality, we observe that for all $n_k>N$,

$$
\begin{aligned}
&\left\|\left|\varphi_{n_k}\right|^2-|\varphi|^2\right\|_{L^{6/5}(\{|x|\leq R\})} \\
&\quad\leq\left\|\left|\varphi_{n_k}\right|+|\varphi|\right\|_{L^{12/5}(\{|x|\leq R\})}\left\|\left|\varphi_{n_k}\right|-|\varphi|\right\|_{L^{12/5}(\{|x|\leq R\})}
\end{aligned}
$$

$$
\leq\left(\left\|\varphi_{n_k}\right\|_{\frac{12}{5}}+\|\varphi\|_{\frac{12}{5}}\right)\left\|\varphi_{n_k}-\varphi\right\|_{L^{12/5}(\{|x|\leq R\})}<C\epsilon. \tag{5.1.42}
$$

Likewise, from the uniform bound in (5.1.24) and the bounds in (5.1.32) and (5.1.33) above, for all $n_k>N$

$$
\left\|\left|\varphi_{n_k}\right|^2-|\varphi|^2\right\|_{L^{6/5}(\{|x|>R\})}
$$

$$\leq \left(\left\|\varphi_{n_k}\right\|_{\frac{12}{5}} + \|\varphi\|_{\frac{12}{5}}\right)\left\|\varphi_{n_k} - \varphi\right\|_{L^{12/5}(\{|x|>R\})}$$

$$\leq \left(\left\|\varphi_{n_k}\right\|_{\frac{12}{5}} + \left\|\varphi_{n_k}\right\|_{\frac{12}{5}}\right)\left\|\varphi_{n_k} - \varphi\right\|_{L^2(\{|x|>R\})}^{\frac{5}{12}}\left\|\varphi_{n_k} - \varphi\right\|_{L^{14/5}(\{|x|>R\})}^{\frac{7}{12}}$$

$$\leq \left(\left\|\varphi_{n_k}\right\|_{\frac{12}{5}} + \left\|\varphi_{n_k}\right\|_{\frac{12}{5}}\right)\left(\left\|\varphi_{n_k}\right\|_{L^{14/5}(\{|x|>R\})} + \|\varphi\|_{L^{14/5}(\{|x|>R\})}\right)^{\frac{7}{12}}\left\|\varphi_{n_k} - \varphi\right\|_{L^2(\{|x|>R\})}^{\frac{5}{12}}$$

$$(5.1.43)\quad \leq C\left(\left\|\varphi_{n_k}\right\|_{L^2(\{|x|>R\})} + \|\varphi\|_{L^2(\{|x|>R\})}\right)^{\frac{5}{12}} < C\left(2\sqrt{\epsilon}\right)^{\frac{5}{12}}.$$

Since $\epsilon$ is arbitrary, the weak continuity in (5.1.40) of the Coulomb energy follows from (5.1.41), (5.1.42) and (5.1.43).

**Step 5** (Weak Limit is a Minimizer). Using the above Lemma, we have established in (5.1.26) that $\|\varphi\|_2 = 1$. Then, from the weak lower semicontinuity of the kinetic energy (5.1.22) and the weak continuity of the potential (5.1.28) and Coulomb (5.1.40) energies, we see

$$e(V) = \liminf_{k\to\infty} \mathcal{E}_V\left(\varphi_{n_k}\right) \geq \mathcal{E}_V(\varphi) \geq e(V).$$

Therefore, the weak limit $\varphi \in H^1(\mathbb{R}^3)$ is a minimizer:

$$(5.1.44)\qquad \mathcal{E}_V(\varphi) = e(V).$$

**Step 6** (Relative Compactness of Minimizing Sequence in $H^1$). We have already argued in (5.1.26) using the above Lemma that $\left\|\varphi_{n_k} - \varphi\right\|_2 \to 0$. Furthermore, for all $k$

$$\left\|\nabla\varphi_{n_k}\right\|_2^2 = \mathcal{E}_V\left(\varphi_{n_k}\right) + \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\varphi_{n_k}(x)\right|^2\left|\varphi_{n_k}(y)\right|^2}{|x-y|}dx\,dy + \int_{\mathbb{R}^3} V(x)\left|\varphi_{n_k}(x)\right|^2 dx.$$

Since $\left\{\varphi_{n_k}\right\}_{k=1}^{\infty}$ is a minimizing sequence and $\varphi(x)$ is a minimizer for the energy $e(V)$,

$$\lim_{k\to\infty}\left\|\nabla\varphi_{n_k}\right\|_2^2 = e(V) + \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\varphi(x)|^2|\varphi(y)|^2}{|x-y|}dx\,dy + \int_{\mathbb{R}^3} V(x)|\varphi(x)|^2 dx.$$
$$= \|\nabla\varphi\|_2^2.$$

Because $\varphi_{n_k} \rightharpoonup \varphi$ in $H^1(\mathbb{R}^3)$ and $\left\|\nabla\varphi_{n_k}\right\|_2 \to \|\nabla\varphi\|_2$, we have $\left\|\nabla\varphi_{n_k} - \nabla\varphi\right\|_2 \to 0$. Hence,

$$\left\|\varphi_{n_k} - \varphi\right\|_{H^1(\mathbb{R}^3)} \to 0.$$

□

We have shown that for each $R > 2$, the Pekar minimization problems $e(V_R)$ admit minimizers. Furthermore, for each $R \geq 2$ let us define the radial minimization problem

$$(5.1.45)\qquad e_R^{\text{rad}} = \inf\left\{\mathcal{E}_{V_R}(\phi) \mid \phi \in H^1_{\text{rad}}(\mathbb{R}^3),\ \|\phi\|_2 = 1\right\}.$$

Essential to our proof of the fact that the minimizers for $e(V_R)$ (for $R$ sufficiently large) admit a non-radial minimizer is that the radial minimization problem in (5.1.45) has a minimizer.

Lemma 32. *For each $R \geq 2$, the radial minimization problem $e_R^{rad}$ admits a minimizer.*

Proof. Lemma II.2 in [**Ls1981**].

□

We do not provide the proof, because it has been given by Lions in 1981 [**Ls1981**], and it is very similar to the compactness argument used in the proof of the nonradiality of the Pekar minimizers. The essential idea is that a radial minimizing sequence $\{\varphi_n\}_n$ that is uniformly bounded in $H^1(\mathbb{R}^3)$ decays uniformly, i.e., for all $n$ and $|x| \geq 1$, $|\varphi_n(x)| \leq C|x|^{-1}$ (see "Radial Lemma 1" in [**Ss1977**] and cf. Theorem II.1 in [**Ls1981**]). This can be seen as follows: We utilize the following observation of W. Strauss (cf. "Radial Lemma 1" in [**Ss1977**] for a general statement): If $u \in H^1(\mathbb{R}^3)$ is a radial function, then

$$|u(x)| \leq \frac{\sqrt{2}\,|\mathbb{S}^2|^{-\frac{1}{2}}\,\|u\|_{H^1(\mathbb{R}^3)}}{|x|} \quad \text{for almost every} \quad |x| \geq 2. \tag{5.1.46}$$

It follows from the simple fact that for any radial $u(x) \in C_c^\infty(\mathbb{R}^3) \cap H^1(\mathbb{R}^3)$, denoting $u(x) = \nu(|x|)$,

$$\left(r^2\nu^2\right)_r = 2\,(r\nu)_r\,(r\nu) \leq (r\nu)_r^2 + (r\nu)^2 = r^2\left(\nu_r^2 + \nu^2\right) + \left(r\nu^2\right)_r.$$

Then, for all $R \geq 2$,

$$\frac{\nu^2(R)}{2}R^2 \leq \nu^2(R)\left(R^2 - R\right) \leq \int_0^R \left(\nu_r^2 + v^2\right) r^2\,dr \leq \left|\mathbb{S}^2\right|^{-1}\|\nu\|_{H^1}^2.$$

A standard density argument shows (5.1.46) for any $u \in H^1(\mathbb{R}^3)$. This observation of Strauss will be crucial also for establishing nonradiality by proving:

Theorem 33. *Let the potential $V_R(x)$ be as given above , and let the energies $e(V_R)$ and $e^{rad}(V_R)$ be as defined by the minimization problems above. Then there exists some $R_* \geq 2$ such that for all $R > R_*$,*

$$e(V_R) < e^{rad}(V_R). \tag{5.1.47}$$

Proof. Essential to the proof is an analysis of the free Pekar problem (i.e., without an external potential):

**Step 1** (Free Minimization Problem). Recall that the Free Minimization Problem

$$e(0) = \inf_{\|\psi\|_2=1} \mathcal{E}_0(\psi) \tag{5.1.48}$$

with

$$\mathcal{E}_0(\psi) = \int_{\mathbb{R}^3} |\nabla\psi|^2 dx - \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\psi(x)|^2\,|\psi(y)|^2}{|x-y|}dx\,dy \tag{5.1.49}$$

admits a symmetric decreasing minimizer (Theorem 7 in **[Lb1977]**), which we shall denote as $Q(x) \in H^1(\mathbb{R}^3)$. We consider the translated functions

$$Q_R(x) = Q\left(x_1 - \left(\frac{R+2}{2}\right),\, x_2,\, x_3\right), \tag{5.1.50}$$

which sit in the potential well at $\{2 \le |x| \le R\}$ when $R$ is large. Since the Free Pekar Functional defined in (5.1.49) is invariant under translations,

$$\mathcal{E}_0(Q_R) = \mathcal{E}_0(Q) = e(0) \quad \text{for all } R.$$

These translated functions $Q_R(x)$ in (5.1.50) will serve as a benchmark for proving the inequality in (5.1.47):

**Step 2** (Variational Principle). It follows from the variational principle that for all $R \geq 2$,

$$e(V_R) \le \mathcal{E}_{V_R}(Q_R) = e(0) - \int_{\mathbb{R}^3} V_R(x)\,|Q_R(x)|^2\,dx. \tag{5.1.51}$$

We also know from the above lemma that for each $R \geq 2$, there exists a radial function $\rho_R \in H^1(\mathbb{R}^3)$, $\|\rho_R\|_2 = 1$ such that $\mathcal{E}_{V_R}(\rho_R) = e^{\mathrm{rad}}(V_R)$. It then suffices to argue that there exists some $R_* \geq 2$ such that

$$\mathcal{E}_{V_R}(Q_R) < \mathcal{E}_{V_R}(\rho_R) \quad \text{for all } R > R_*. \tag{5.1.52}$$

**Step 3** (Proof by Contradiction). We shall prove (5.1.52) by contradiction. Suppose for each $R_* \geq 2$ there is some $R > R_*$ such that $\mathcal{E}_{V_R}(Q_R) \geq \mathcal{E}_{V_R}(\rho_R)$. Then we can extract a sequence $\{R_n\}_{n=1}^{\infty}$ where $R_n \to \infty$ as $n \to \infty$ and for all $n$,

$$e(0) - \int_{\mathbb{R}^3} V_{R_n}(x)\left|Q_{R_n}(x)\right|^2 dx \geq \mathcal{E}_0\left(\rho_{R_n}\right) - \int_{\mathbb{R}^3} V_{R_n}(x)\left|\rho_{R_n}(x)\right|^2 dx. \tag{5.1.53}$$

From (5.1.53) and observing from the variational principle that $\mathcal{E}_0\left(\rho_{R_n}\right) \geq e(0)$, we then have for all $n$,

$$0 \le \mathcal{E}_0\left(\rho_{R_n}\right) - e(0) \le \int_{\mathbb{R}^3} V_{R_n}(x)\left|\rho_{R_n}(x)\right|^2 dx - \int_{\mathbb{R}^3} V_{R_n}(x)\left|Q_{R_n}(x)\right|^2 dx. \tag{5.1.54}$$

**Step 4** (Radial Minimizers Live in Potential Well). Since $V_{R_n}(x) = 1$ for $2 \le |x| \le R_n$ and $0 \le V_{R_n}(x) \le 1$, it follows from our observation in (5.1.54) and Hölder's inequality that for all $n$,

$$\int_{\{2 \le |x| \le R_n\}} \left|Q_{R_n}(x)\right|^2 dx \le \int_{\mathbb{R}^3} V_{R_n}(x)\left|Q_{R_n}(x)\right|^2 dx \le \int_{\mathbb{R}^3} V_{R_n}(x)\left|\rho_{R_n}(x)\right|^2 dx \le 1. \tag{5.1.55}$$

Furthermore, $\|Q\|_2 = 1$ and for any $\epsilon > 0$ there is a $K_\epsilon > 0$ such that

$$\int_{\{|x| < K_\epsilon\}} |Q(x)|^2\,dx > 1 - \epsilon.$$

Denoting the vector $\mathbf{v}_n = \left(\frac{R_n+2}{2},\, 0,\, 0\right)$, it follows from the definition of $Q_{R_n}(x)$ given in (5.1.50) that for all $n$,

$$\int_{\{|x - \mathbf{v}_n| < K_\epsilon\}} \left|Q_{R_n}(x)\right|^2 dx > 1 - \epsilon;$$

in particular, $K_\epsilon$ does not depend on $n$. Since $R_n \to \infty$, there exists some $N$ such that for all $n > N$
$$\{|x - \mathbf{v}_n| < K_\epsilon\} \subseteq \{2 \le |x| \le R_n\}.$$
Then for $n > N$,
$$1 - \epsilon \le \int_{\{|x-\mathbf{v}_n|<K_\epsilon\}} \left|Q_{R_n}(x)\right|^2 dx \le \int_{\{2\le|x|\le R_n\}} \left|Q_{R_n}(x)\right|^2 dx \le 1.$$
Since $\epsilon > 0$ is arbitrary,
$$\lim_{n\to\infty} \int_{\{2\le|x|\le R_n\}} \left|Q_{R_n}(x)\right|^2 dx = 1. \tag{5.1.56}$$
From (5.1.55) and (5.1.56) we have
$$\lim_{n\to\infty} \int_{\mathbb{R}^3} V_{R_n}(x) \left|\rho_{R_n}(x)\right|^2 dx = 1. \tag{5.1.57}$$
For all $n$, $\|\rho_{R_n}\|_2 = 1$, $0 \le V_{R_n}(x) \le 1$ and $V_{R_n}(x) = 0$ when $|x| \le 1$, so
$$\int_{\mathbb{R}^3} V_{R_n}(x) \left|\rho_{R_n}(x)\right|^2 dx \le \int_{\mathbb{R}^3} \left|\rho_{R_n}(x)\right|^2 dx \le 1. \tag{5.1.58}$$
Then, from (5.1.57) and (5.1.58) we observe that
$$\lim_{n\to\infty} \int_{\{|x|>1\}} \left|\rho_{R_n}(x)\right|^2 dx = 1.$$
Since $\|\rho_{R_n}\|_2 = 1$, we have to conclude that
$$\lim_{n\to\infty} \int_{\{|x|\le1\}} \left|\rho_{R_n}(x)\right|^2 dx = 0. \tag{5.1.59}$$

**Step 5** (Radial Minimizers are Minimizing for the Free Problem). Since, for all $n$, $0 \le V_{R_n}(x) \le 1$ and $V_{R_n}(x) = 1$ when $2 \le |x| \le R_n$, it follows from (5.1.56) that
$$\lim_{n\to\infty} \int_{\mathbb{R}^3} V_{R_n}(x) \left|Q_{R_n}(x)\right|^2 dx = 1.$$
From (5.1.54) and (5.1.57) we then have to conclude that
$$\lim_{n\to\infty} \mathcal{E}_0\left(\rho_{R_n}\right) = e(0). \tag{5.1.60}$$
We are now ready to produce a contradiction:

**Step 6** (Contradiction). The *radial* sequence $\left\{\rho_{R_n}\right\}_{n=1}^\infty \in H^1(\mathbb{R}^3)$, $\|\rho_{R_n}\|_2 = 1$ satisfying (5.1.59) is a minimizing sequence for the Free Pekar Energy $e(0)$ given in (5.1.48) above, and we proceed in the usual way to extract a weak limit. For $u \in H^1(\mathbb{R}^3)$, $\|u\|_2 = 1$ we again recall the Sobolev inequality, $\|\nabla u\|_2^2 \ge S\|u\|_6^2$ with the best constant $S = 3(\pi/2)^{4/3}$. Writing $|x|^{-1} = h_{1;\beta}(x) + h_{2;\beta}(x)$, where
$$h_{1;\beta}(x) = |x|^{-1}\chi^{(x)}_{\{|x|\le\beta\}} \quad \text{and} \quad h_{2;\beta}(x) = |x|^{-1}\chi^{(x)}_{\{|x|>\beta\}},$$
we choose $\beta$ small so that
$$\|h_{1;\beta}\|_{\frac{3}{2}} = (4\pi)^{\frac{2}{3}}\beta^{\frac{1}{3}} < \frac{S}{2}.$$

We now observe using the Sobolev and Young's inequalities that for any $u \in H^1(\mathbb{R}^3)$ and $\|u\|_2 = 1$,

$$\begin{aligned}\mathcal{E}_0(u) &\geq \|\nabla u\|_2^2 - \|h_{1;\beta}\|_{\frac{3}{2}} \|u\|_6^2 - \beta^{-1} \\ &\geq \|\nabla u\|_2^2 \left(1 - \frac{\|h_{1;\beta}\|_{\frac{3}{2}}}{S}\right) - \beta^{-1} \\ &\geq \frac{\|\nabla u\|_2^2}{2} - \beta^{-1} \qquad (5.1.61) \\ &\geq -\beta^{-1} > -\infty.\end{aligned}$$

Therefore, $e(0) > -\infty$. Moreover, $e(0) < 0$ (cf. Lemma 1 (i) in [**Lb1977**]; this follows from a Gaussian trial function.). Then for $n$ large,

$$\mathcal{E}_0\left(\rho_{R_n}\right) < e(0) + 1 < 1,$$

and we observe from (5.1.61) that (for $n$ large),

$$\left\|\nabla \rho_{R_n}\right\|_2^2 \leq 2\left(\mathcal{E}_0\left(\rho_{R_n}\right) + \beta^{-1}\right) < 2\left(1 + \beta^{-1}\right).$$

Since $\left\|\rho_{R_n}\right\|_2 = 1$, for $n$ large

$$\|\rho_{R_n}\|_{H^1(\mathbb{R}^3)} < C. \qquad (5.1.62)$$

With (5.1.62) we conclude that there exists a (radial) subsequence $\left\{\rho_{R_{n_k}}\right\}_{k=1}^{\infty}$, $\left\|\rho_{R_{n_k}}\right\|_2 = 1$ (satisfying (5.1.59)) and some $\rho \in H^1(\mathbb{R}^3)$, where

$$\rho_{R_{n_k}} \rightharpoonup \rho \ \text{ in } \ H^1\left(\mathbb{R}^3\right). \qquad (5.1.63)$$

We begin with some immediate consequences of the weak convergence in (5.1.63). From the weak lower semicontinuity of the $L^2$-norm we have

$$\|\rho\|_2 \leq \liminf_{k\to\infty} \left\|\rho_{R_{n_k}}\right\|_2 = 1, \qquad (5.1.64)$$

and

$$\|\nabla\rho\|_2 \leq \liminf_{k\to\infty} \left\|\nabla\rho_{R_{n_k}}\right\|_2. \qquad (5.1.65)$$

Furthermore, the sequence $\left\{\rho_{R_{n_k}}\right\}_{k=1}^{\infty}$ is radial, and therefore the weak limit $\rho(x)$ is radial almost everywhere. Finally, it follows from the Rellich-Kondrashov theorem (Theorem 8.6 in [**LL2001**]) and (5.1.59) that

$$\int_{\{|x|\leq 1\}} |\rho(x)|^2\, dx = \lim_{k\to\infty} \int_{\{|x|\leq 1\}} \left|\rho_{R_{n_k}}(x)\right|^2 dx = 0. \qquad (5.1.66)$$

(That $\rho(x)$ is radial almost everywhere and satisfies the property in (5.1.66) above will be crucial for arriving at a contradiction, as we shall soon see.)

The subsequence of radial functions $\{\rho_{n_k}\}_{k=1}^{\infty}$ is uniformly bounded in $H^1(\mathbb{R}^3)$ (see (5.1.62) above), so it follows from an observation of Strauss given above in (5.1.46) (see "Radial Lemma 1" in [**Ss1977**]) that, for all $k$ and some constant $C > 0$

$$\left|\rho_{R_{n_k}}(x)\right| < \frac{C}{|x|} \ \text{ for almost every } \ |x| \geq 2. \qquad (5.1.67)$$

Denoting for $\epsilon > 0$ the sets

$$A_\epsilon := \left\{ x \in \mathbb{R}^3 \mid \left|\rho_{R_{n_k}}(x)\right| \geq \epsilon \ \text{ for all } \ \mathrm{k} \right\} \tag{5.1.68}$$

and

$$B_\epsilon := \left\{ x \in \mathbb{R}^3 \mid |x| \leq \frac{C}{\epsilon} \right\},$$

we deduce from (5.1.67) that for any $\epsilon > 0$,

$$|A_\epsilon| \leq |B_\epsilon| = \frac{4\pi C^3}{3\epsilon^3} < \infty. \tag{5.1.69}$$

We now argue the weak continuity of the Coulomb energy: that as $k \to \infty$,

$$\left| \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\rho_{R_{n_k}}(x)\right|^2 \left|\rho_{R_{n_k}}(y)\right|^2}{|x-y|} dx\, dy - \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\rho(x)|^2\, |\rho(y)|^2}{|x-y|} dx\, dy \right| \longrightarrow 0. \tag{5.1.70}$$

For any $\epsilon > 0$, let the set $A_\epsilon$ be as given in (5.1.68), and let $A_\epsilon^C$ denote its complement in $\mathbb{R}^3$. It follows from the positivity of the Coulomb energy (Theorem 9.8 in [**LL2001**]) and the Hardy-Littlewood-Sobolev inequality that

$$\left| \left( \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{\left|\rho_{R_{n_k}}(x)\right|^2 \left|\rho_{R_{n_k}}(y)\right|^2}{|x-y|} dx\, dy \right)^{\frac{1}{2}} - \left( \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|\rho(x)|^2\, |\rho(y)|^2}{|x-y|} dx\, dy \right)^{\frac{1}{2}} \right|$$

$$\leq C_{\mathrm{HLS}}^{1/2} \left( \left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^{6/5}(A_\epsilon)} + \left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^{6/5}(A_\epsilon^C)} \right). \tag{5.1.71}$$

As we have argued in (5.1.42) above, it follows from Hölder's inequality that

$$\left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^{6/5}(A_\epsilon)} \leq \left( \left\|\rho_{R_{n_k}}\right\|_{\frac{12}{5}} + \|\rho\|_{\frac{12}{5}} \right) \left\|\rho_{R_{n_k}} - \rho\right\|_{L^{12/5}(A_\epsilon)}. \tag{5.1.72}$$

Since the sequence $\left\{\rho_{R_{n_k}}\right\}_{k=1}^{\infty}$ is uniformly bounded in $H^1(\mathbb{R}^3)$ (see (5.1.62) above), it follows from the Sobolev inequality and the weak lower semicontinuity of the $L^p$-norm that $\left\|\rho_{R_{n_k}}\right\|_{12/5} < C$ for all $k$ and $\rho \in L^{12/5}(\mathbb{R}^3)$. Since $|A_\epsilon| < \infty$ (see (5.1.69) above), we deduce from the Rellich-Kondrashov theorem (Theorem 8.6 in [**LL2001**]) that $\left\|\rho_{R_{n_k}} - \rho\right\|_{L^{12/5}(A_\epsilon)} \to 0$ as $k \to \infty$. From (5.1.72) we conclude that

$$\left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^{6/5}(A_\epsilon)} \longrightarrow 0 \ \text{ as } \ k \to \infty. \tag{5.1.73}$$

Finally, we recall from (5.1.64) that $\|\rho\|_2 \leq 1$ and again observe using Hölder's inequality that

$$\left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^{6/5}(A_\epsilon^C)} \leq \left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^\infty(A_\epsilon^C)}^{1/6} \left\| \left|\rho_{R_{n_k}}\right|^2 - |\rho|^2 \right\|_{L^1(A_\epsilon^C)}^{5/6}$$

$$\leq 2^{\frac{5}{6}} \left( \left\| \rho_{R_{n_k}} \right\|^2_{L^\infty(A^C_\epsilon)} + \|\rho\|^2_{L^\infty(A^C_\epsilon)} \right)^{\frac{1}{6}}. \tag{5.1.74}$$

From the definition of $A_\epsilon$ given in (5.1.68) above we know that $\left\| \rho_{R_{n_k}} \right\|_{L^\infty(A^C_\epsilon)} < \epsilon$. Furthermore, since $\rho_{R_{n_k}} \rightharpoonup \rho$ in $H^1(\mathbb{R}^3)$, we also know that $\rho_{R_{n_k}}$ converges to $\rho$ pointwise almost everywhere (Corollary 8.7 in [**LL2001**]). Therefore, $\|\rho\|_{L^\infty(A^C_\epsilon)} < \epsilon$ and we now see from (5.1.74) that

$$\left\| \left| \rho_{R_{n_k}} \right|^2 - |\rho|^2 \right\|_{L^{6/5}(A^C_\epsilon)} < 2\epsilon^{\frac{1}{3}}. \tag{5.1.75}$$

Since $\epsilon > 0$ is arbitrary, the weak continuity of the Coulomb energy in (5.1.70) follows from (5.1.71), (5.1.73) and (5.1.75).

Since $\|\rho\|_2 \leq 1$ (see (5.1.64) above) and $e(0) < 0$ (Lemma 1(i) in [**Lb1977**]), we observe that

$$\mathcal{E}_0(\rho) \geq e(0) \|\rho\|^2_2 \geq e(0). \tag{5.1.76}$$

It also follows from (5.1.65) and (5.1.70) that

$$e(0) = \liminf_{k\to\infty} \mathcal{E}_0\left(\rho_{R_{n_k}}\right) \geq \mathcal{E}_0(\rho). \tag{5.1.77}$$

From (5.1.76) and (5.1.77) we conclude

$$\|\rho\|_2 = 1 \quad \text{and} \quad \mathcal{E}_0(\rho) = e(0). \tag{5.1.78}$$

Let us summarize: If there does not exist some $R_* \geq 2$ such that $\mathcal{E}_{V_R}(Q_R) < \mathcal{E}_{V_R}(\rho_R)$ for all $R > R_*$ (see (5.1.52) above), then we can extract a radial sequence $\left\{\rho_{R_{n_k}}\right\}_{k=1}^{\infty}$ that converges weakly in $H^1(\mathbb{R}^3)$ to $\rho$, which (as we have argued in (5.1.78)) is a minimizer for the Free Minimization Problem in (5.1.48). Furthermore, it is known that the minimization problem in (5.1.48) admits a symmetric decreasing minimizer $Q(x)$, which is, up to translations, the *unique* minimizer (Theorem 10 in [**Lb1977**]). We are then forced to conclude that

$$\rho(x) = Q(x-a), \quad \text{some} \;\; a \in \mathbb{R}^3. \tag{5.1.79}$$

Since the weak limit $\rho(x)$ is radial almost everywhere, $a = 0$ necessarily in (5.1.79) above, and $\rho(x) = Q(x)$, which is symmetric decreasing about the origin. However, we observe from (5.1.66) that $\rho(x) = 0$ for almost every $|x| \leq 1$, and this is a contradiction.

**Step 7** (Conclusion). We have argued by contradiction that there exists some $R_* \geq 2$ such that $\mathcal{E}_{V_R}(Q_R) < \mathcal{E}_{V_R}(\rho_R)$ for all $R > R_*$. From the variational principle and that $\mathcal{E}_{V_R}(\rho_R) = e^{\text{rad}}(V_R)$, for all $R > R_*$

$$e_R \leq \mathcal{E}_{V_R}(Q_R) < \mathcal{E}_{V_R}(\rho_R) = e^{\text{rad}}(V_R),$$

which proves the Theorem.

□

Remark. The above theorem clearly shows that for $R$ large, a minimizer for the Pekar energy $e_R$ is not radial. In fact, since $V_R(x)$ is a radial function and the Pekar functional

$\mathcal{E}_{V_R}(\cdot)$ is invariant under rotations, each rotation of the non-radial minimizer also minimizes the functional. The minimizer for the problem $e(V_R)$ is therefore not unique. To our knowledge, this is the first non-uniqueness result for the Pekar functional with an external potential. The uniqueness of a minimizer in the presence of an external potential, however, remains an elusive open problem.

## 5.2. Convergence to the Rotational Average

In order to prove anything about the convergence of the ground-state electron density one has to perturb the Pekar energy and differentiate. Differentiation for all $C_c^\infty$ perturbations is not possible without uniqueness. However, it is possible to differentiate with radial perturbations when the minimizer is unique up to rotation!

THEOREM 34. *For $W \in L^{3/2}(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$ and a real parameter $\delta$ consider the perturbed Pekar energy*

$$e(V_R+\delta W) = \inf_{\|u\|_2=1} \mathcal{E}_{V_R+\delta W}(u) = \inf_{\|u\|_2=1} \left\{ \mathcal{E}_{V_R}(u) - \delta \int_{\mathbb{R}^3} |u(x)|^2 W(x)\, dx \right\} \tag{5.2.1}$$

*where*

$$\mathcal{E}_{V_R}(u) = \int_{\mathbb{R}^3} |\nabla u|^2 dx - \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|u(x)|^2\,|u(y)|^2}{|x-y|} dx\, dy - \int_{\mathbb{R}^3} V_R(x)|u(x)|^2 dx.$$

*Suppose the minimization problem for the Pekar energy $e(V_R) = \inf\{\mathcal{E}_{V_R}(u) : \ \|u\|_2 = 1\}$ admits a minimizer $u_{V_R}$ that is unique up to rotations. For radial $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ the map $\delta \mapsto e(V_R+\delta Z)$ is differentiable at $\delta = 0$, and*

$$\left.\frac{d}{d\delta}\right|_{\delta=0} e(V_R+\delta Z) = -\int_{\mathbb{R}^3} |u_{V_R}(x)|^2 Z(x)\, dx. \tag{5.2.2}$$

PROOF. For any $W \in L^{3/2}(\mathbb{R}^3)+L^\infty(\mathbb{R}^3)$, by a standard argument (**[Lb1977]**, **[LL2001]**) using Sobolev's and Young's inequalities, there exist constants $0 < c_1 < 1$ and $c_2 > 0$ such that for all $u \in H^1(\mathbb{R}^3)$ with $\|u\|_2 = 1$ and $|\delta|$ sufficiently small,

$$\mathcal{E}_{V_R+\delta W}(u) \geq c_1 \|\nabla u\|_2^2 - c_2. \tag{5.2.3}$$

Therefore,

$$e(V_R+\delta W) > -\infty. \tag{5.2.4}$$

We deduce from (5.2.4) that for $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ (and $|\delta|$ sufficiently small), the perturbed problem $e(V+\delta W)$ admits an approximate minimizer $u_\delta \in H^1(\mathbb{R}^3)$ with $\|u_\delta\|_2 = 1$ satisfying

$$\mathcal{E}_{V_R+\delta W}(u_\delta) \leq e(V_R+\delta W) + \delta^2. \tag{5.2.5}$$

We denote the set of minimizers for the Pekar energy as $\mathcal{M} := \{u \in H^1(\mathbb{R}^3) : \ \|u\|_2 = 1 \text{ and } \mathcal{E}_{V_R}(u) = e(V_R)\}$. For any $\tilde{u} \in \mathcal{M}$, by the variational principle,

$$e(V_R+\delta W) \leq \mathcal{E}_{V_R+\delta W}(\tilde{u}) = e(V_R) - \delta \int_{\mathbb{R}^3} W(x)|\tilde{u}(x)|^2 dx. \tag{5.2.6}$$

Likewise, for an approximate minimizer $u_\delta$, $\|u_\delta\|_2 = 1$ satisfying (5.2.5),

$$e(V) \le \mathcal{E}_{V_R}(u_\delta) = \mathcal{E}_{V_R+\delta W}(u_\delta) + \delta \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx$$

$$\le e(V_R + \delta W) + \delta^2 + \delta \int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx. \tag{5.2.7}$$

Let $\delta > 0$. For a perturbation $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ and an approximate minimizer $u_\delta$, $\|u_\delta\|_2 = 1$ in (5.2.5), by the inequalities in (5.2.6) and (5.2.7),

$$-\int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx - \delta \le \frac{e(V+\delta W) - e(V)}{\delta} \le -\left(\sup_{u\in\mathcal{M}} \int_{\mathbb{R}^3} W(x)|u(x)|^2 dx\right). \tag{5.2.8}$$

When $\delta < 0$, the inequalities in (5.2.8) are merely reversed:

$$-\int_{\mathbb{R}^3} W(x)|u_\delta(x)|^2 dx - \delta \ge \frac{e(V+\delta W) - e(V)}{\delta} \ge -\left(\inf_{u\in\mathcal{M}} \int_{\mathbb{R}^3} W(x)|u(x)|^2 dx\right). \tag{5.2.9}$$

By our uniqueness assumption, $\mathcal{M} = \{u_V(\mathcal{R}x) : \mathcal{R} \in SO(3)\}$. Furthermore, with radial functions $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, by a change of variable,

$$\int_{\mathbb{R}^3} Z(x)|u_{V_R}(\mathcal{R}x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_{V_R}(x)|^2 dx \tag{5.2.10}$$

for all $\mathcal{R} \in SO(3)$. Then, for radial perturbations, the rightmost quantities in the inequalities (5.2.8) and (5.2.9) are equal. Hence (with $Z$ radial) the claimed differentiability of the map $\delta \mapsto e(V_R + \delta W)$ at $\delta = 0$ will follow from our observation in (5.2.10) and the inequalities in (5.2.8) and (5.2.9) if we can prove the convergence result stated below:

For radial $Z \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$, let $u_\delta$ with $\|u_\delta\|_2 = 1$ be an approximate minimizer as defined in (5.2.5) above for the perturbed energy $e(V_R + \delta Z)$. Then, for any sequence $\{\delta_n\}_{n=1}^\infty$ where $|\delta_n| > 0$ and $\delta_n \to 0$ as $n \to \infty$, the corresponding sequence of approximate minimizer $\{u_{\delta_n}\}_{n=1}^\infty$ satisfies

$$\lim_{n\to\infty} \int_{\mathbb{R}^3} Z(x)|u_{\delta_n}(x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_{V_R}(x)|^2 dx. \tag{5.2.11}$$

We observe that $\{u_{\delta_n}\}_{n=1}^\infty$ is minimizing for the problem $e(V_R) = \inf\{\mathcal{E}_{V_R}(u) : \|u\|_2 = 1\}$. Then, by the compactness argument given in the above section, every subsequence $\{u_{\delta_{n_k}}\}$ has a sub-subsequence $\{u_{\delta_{n_{k_l}}}\}$ converging strongly in $H^1(\mathbb{R}^3)$ to some function in $\mathcal{M} = \{u_{V_R}(\mathcal{R}x) : \mathcal{R} \in \mathcal{S}O(3)\}$. We deduce from our observation in (5.2.10) that

$$\lim_{l\to\infty} \int_{\mathbb{R}^3} Z(x)|u_{\delta_{n_{k_l}}}(x)|^2 dx = \int_{\mathbb{R}^3} Z(x)|u_{V_R}(\mathcal{R}x)|^2 dx$$

$$= \int Z(x)|u_V(x)|^2 dx.$$

Since every subsequence converges, (5.2.11) holds.

□

Now we prove Theorem 29

Proof of Theorem 29. For any $W \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$ we denote its rotational average $\langle W \rangle = \int_{SO(3)} W(\mathcal{R}x)\, d\gamma(\mathcal{R})$. Note that $\langle W \rangle \in L^{3/2}(\mathbb{R}^3) + L^\infty(\mathbb{R}^3)$. As explained in the introduction, using the variational principle and (5.0.16), we arrive at the relations

$$\frac{e(V_R+\delta\langle W\rangle)-e(V_R)}{\delta}\leq \liminf_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\langle W\rangle(x)\,dx,$$

and

$$\frac{e(V_R+\delta\langle W\rangle)-e(V_R)}{\delta}\geq \limsup_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\langle W\rangle(x)\,dx.$$

Using Fubini's theorem, a simple change of variable and that the electron density $\|\Psi_\alpha^V\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)$ is radial, we observe

$$\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\langle W\rangle(x)\,dx=\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)W(x)\,dx. \tag{5.2.12}$$

Furthermore, since $\langle W\rangle$ is radial and we assume that the problem in (5.0.14) admits a minimizer $u_{V_R}$ that is unique up to rotations, we conclude from Theorem 34 and (5.2.12):

$$\begin{aligned}\lim_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)W(x)\,dx &= \lim_{\alpha\to\infty} -\frac{1}{\alpha^3}\int_{\mathbb{R}^3}\|\Psi_\alpha^{V_R}\|_{\mathcal{F}}^2\left(\frac{x}{\alpha}\right)\langle W\rangle(x)\,dx\\ &= \left.\frac{d}{d\delta}\right|_{\delta=0} e(V_R+\delta\langle W\rangle)\\ &= -\int_{\mathbb{R}^3}|u_{V_R}(x)|^2\langle W\rangle(x)\,dx\\ &= -\int_{\mathbb{R}^3}\left(\int_{SO(3)}|u_{V_R}(\mathcal{R}x)|^2 d\gamma(\mathcal{R})\right)W(x)\,dx.\end{aligned}$$

□

## 5.3. A Calculation with the Rotational Average

Recall the Pekar Ansatz for the Hamiltonian $H_\alpha(V_R)$ considered above,

$$\Psi=\alpha^{3/2}\phi_{V_R}(\alpha x)\Phi$$

where

$$\Phi=\prod_k \exp\left(\frac{z_\alpha(k)}{|k|}a_k^\dagger-\frac{\overline{z_\alpha(k)}}{|k|}a_k\right)|0\rangle$$

and

$$z_\alpha(k)=\frac{1}{\pi}\sqrt{\frac{\alpha}{2}}\int_{\mathbb{R}^3}e^{-ik\cdot x}|\alpha^{3/2}\phi_{V_R}(\alpha x)|^2dx, \tag{5.3.1}$$

with $\phi_{V_R}$ the minimizer for the energy $e(V_R)$ described in (5.0.14) and with the Mexican Hat-type potential $V_R$ given in (5.0.2). Here we will provide an amusing calculation which suggested that the ground-state electron density converges to a rotational average of the Pekar minimizers. Here we shall denote the rotational average of Pekar's product wave function as

$$\overline{\Psi}_\rho:=\int_{SO(3)}\Psi_{\mathcal{R}}\,d\gamma(\mathcal{R}),$$

where

$$\Psi_{\mathcal{R}} = \varphi(\mathcal{R}x)\Phi(\mathcal{R}\cdot). \tag{5.3.2}$$

A beautiful calculation yields the following:

LEMMA 35. *Let $\mathcal{R}\mathbf{x}$ denote the rotation of the vector $\mathbf{x} \in \mathbb{R}^3$ by an angle $\theta$ about $\hat{n}$, the axis of rotation. Pekar's coherent state $\Phi_{\mathcal{PK}}$ can be rotated by an angle $\theta$ about $\hat{n}$ as follows:*

$$e^{i\theta\hat{n}\cdot J_f}\Phi_{\mathcal{PK}} = \prod_k \exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(\mathcal{R}k)}{|k|}a_k^\dagger\right)\|0\rangle,$$

*with $J_f = \int_{\mathbb{R}^3} dk(k \times i\nabla_k)a_k^\dagger a_k$ the angular momentum operator relative to the origin.*

To see this, we will use that

$$(a_k^\dagger)^m e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k} = e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\left(e^{i\theta\hat{n}\cdot(k\times i\nabla_k)}\right)^m (a_k^\dagger)^m.$$

and $e^{-i\theta\hat{n}\cdot J_f}\|0\rangle = \|0\rangle$.

PROOF. Note

$$\begin{aligned}
&e^{i\theta\hat{n}\cdot J_f}\prod_k \exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(k)}{|k|}a_k^\dagger\right)\|0\rangle \\
&= e^{i\theta\hat{n}\cdot J_f}\prod_k \exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(k)}{|k|}a_k^\dagger\right)e^{-i\theta\hat{n}\cdot J_f}\|0\rangle \\
&= e^{i\theta\hat{n}\cdot J_f}\prod_k \exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(k)}{|k|}a_k^\dagger\right)e^{-i\theta\hat{n}\cdot J_f}\|0\rangle \\
&= \prod_k e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(k)}{|k|}a_k^\dagger\right)e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\|0\rangle.
\end{aligned}$$

We now evaluate

$$\begin{aligned}
&e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\exp\left(-\tfrac{|z(k)|^2}{2|k|^2} + \tfrac{z(k)}{|k|}a_k^\dagger\right)e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\exp\left(\tfrac{z(k)}{|k|}a_k^\dagger\right)e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\sum_{m=0}^\infty \tfrac{1}{m!}(a_k^\dagger)^m\left(\tfrac{z(k)}{|k|}\right)^m e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\sum_{m=0}^\infty \tfrac{1}{m!}(a_k^\dagger)^m e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\left(\tfrac{z(k)}{|k|}\right)^m\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\sum_{m=0}^\infty \tfrac{1}{m!}e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\left(e^{i\theta\hat{n}\cdot(k\times i\nabla_k)}\right)^m(a_k^\dagger)^m\left(\tfrac{z(k)}{|k|}\right)^m\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)e^{i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\sum_{m=0}^\infty \tfrac{1}{m!}e^{-i\theta\hat{n}\cdot(k\times i\nabla_k)a_k^\dagger a_k}\left(e^{i\theta\hat{n}\cdot(k\times i\nabla_k)}\left(\tfrac{z(k)}{|k|}\right)a_k^\dagger\right)^m\|0\rangle \\
&= \exp\left(-\tfrac{|z(k)|^2}{2|k|^2}\right)\sum_{m=0}^\infty \tfrac{1}{m!}\left(\tfrac{z(\mathcal{R}k)}{|k|}a_k^\dagger\right)^m\|0\rangle
\end{aligned}$$

$= \exp\left(-\frac{|z(k)|^2}{2|k|^2} + \frac{z(\mathcal{R}k)}{|k|}a_k^\dagger\right)\|0\rangle.$

□

Recall that with Pekar's Ansatz $\Psi$ for the wave function (of course the wave function depends on $\alpha$ though we suppressed it for ease of notation)

$$\lim_{\alpha\to\infty}\frac{\langle\Psi, H_\alpha(V_R)\Psi\rangle}{\alpha^2} = e(V_R). \tag{5.3.3}$$

In (5.3.3) $\Psi$ can be replaced with $\Psi_{\mathcal{R}}$ thanks to the rotational invariance of the Hamiltonian. In fact we see that the rotational average of Pekar's wave functions also yield, again to the leading order, the exact ground-state energy

$$\lim_{\alpha\to\infty}\frac{\langle\overline{\Psi}_\rho, H_\alpha(V_R)\overline{\Psi}_\rho\rangle}{\alpha^2\langle\overline{\Psi}_\rho, \overline{\Psi}_\rho\rangle} = e(V_R). \tag{5.3.4}$$

Essential to the calculation is that different rotations of the coherent state (in Fock space) become orthogonal in the strong-coupling limit:

LEMMA 36. *For any $\mathcal{R}, \mathcal{R}' \in SO(3)$,*

$$\lim_{\alpha\to\infty}\langle\Phi(\mathcal{R}\cdot), \Phi(\mathcal{R}'\cdot)\rangle_{\mathcal{F}} = \delta_{\mathcal{R},\mathcal{R}'}.$$

The positivity properties of the Coulomb energy (see Theorem 9.8 in [**LL2001**]) and a mild variation of Corollary 5.10 in [**LL2001**] (a Plancherel-type result for $|x|^{-1}$) play are of the essence in the proof.

PROOF. In the following, $\langle\cdot,\cdot\rangle$ should be read "$\langle\cdot,\cdot\rangle_{\mathcal{F}}$". Let $\mathcal{R} \in SO(3)$. Without loss of generality it suffices for us to show $\lim_{\alpha\to\infty}\langle\Phi(\cdot), \Phi(\mathcal{R}\cdot)\rangle = \delta_{\mathcal{R}(id)}$. We thus calculate:

$$\begin{aligned}
\langle\Phi(\cdot),\, \Phi(\mathcal{R}\cdot)\rangle &= \prod_k \exp\left(-\frac{|z_\varphi(k)|^2}{|k|^2}\right)\left\langle \exp\left(\frac{z_\varphi(k)}{|k|}a_k^\dagger\right)|0\rangle,\ \exp\left(\frac{z_\varphi(\mathcal{R}k)}{|k|}a_k^\dagger\right)|0\rangle\right\rangle \\
&= \prod_k \exp\left(-\frac{|z_\varphi(k)|^2}{|k|^2} + \frac{z_\varphi(k)\overline{z_\varphi}(\mathcal{R}k)}{|k|^2}\right) \\
&= \exp\left(\int_{\mathbb{R}^3}\left(-\frac{|z_\varphi(k)|^2}{|k|^2} + \frac{z(k)\overline{z_\varphi}(\mathcal{R}k)}{|k|^2}\right)dk\right) \\
&= \exp\left(\alpha\left(\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\varphi^2(x)\overline{\varphi^2}(\mathcal{R}y)}{|x-y|}dx\,dy - \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\varphi^2(x)\overline{\varphi^2}(y)}{|x-y|}dx\,dy\right)\right).
\end{aligned}$$

It follows from the positivity of the Coulomb energy that

$$\int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\varphi^2(x)\overline{\varphi^2}(\mathcal{R}y)}{|x-y|}dx\,dy \le \int_{\mathbb{R}^3}\int_{\mathbb{R}^3}\frac{\varphi^2(x)\overline{\varphi^2}(y)}{|x-y|}dx\,dy,$$

and thus $\lim_{\alpha\to\infty}\langle\Phi(\cdot),\, \Phi(\mathcal{R}\cdot)\rangle = 0.$

□

Now seeing (5.3.4) becomes straightforward with the Lemma. Below $\langle\cdot,\cdot\rangle$ should be read as "$\langle\cdot,\cdot\rangle_{L^2(\mathbb{R}^3)\otimes\mathcal{F}}$". In the following, "$\langle\cdot,\cdot\rangle_{\mathcal{F}}$" and "$\langle\cdot,\cdot\rangle_e$" denote the inner product over only the Fock space and electronic coordinates, respectively. First, we observe:

$$\frac{1}{\alpha^2}\frac{\langle\overline{\Psi}_\rho, H_\alpha(V)\overline{\Psi}_\rho\rangle}{\langle\overline{\Psi}_\rho,\overline{\Psi}_\rho\rangle}$$

$$= \frac{1}{\alpha^2}\frac{1}{\langle\overline{\Psi}_\rho,\overline{\Psi}_\rho\rangle}\int\int_{SO(3)\times SO(3)} d\gamma(\mathcal{R})d\gamma(\mathcal{R}')\langle\Psi_{\mathcal{R}'}, H_\alpha(V)\Psi_{\mathcal{R}}\rangle. \tag{5.3.5}$$

Second, using the above Lemma we see that $\lim_{\alpha\to\infty}\langle\overline{\Psi}_\rho,\overline{\Psi}_\rho\rangle = 0$. Below for ease of notation we use $\varphi := \alpha^{3/2}\phi_{V_R}(\alpha x)$. We will also make use of the fact that Pekar's coherent states are eigenstates of the annihlation oeprator, i.e.

$$a_k\Phi(\mathcal{R}\cdot) = z_\alpha(\mathcal{R}k)\Phi(\mathcal{R}\cdot)$$

with $z_\alpha$ as given in (5.3.1) above. In order to evaluate the integrand in (5.3.5), we calculate:

$$\begin{aligned}
&\langle\Psi_{\mathcal{R}'},\ H_\alpha(V)\Psi_{\mathcal{R}}\rangle \\
&= \langle\Psi_{\mathcal{R}'}, p_x^2\Psi_{\mathcal{R}}\rangle + \langle\Psi_{\mathcal{R}'}, \textstyle\int_{\mathbb{R}^3} a_k^\dagger a_k\Psi_{\mathcal{R}}\ dk\rangle \\
&+\alpha^{\frac{1}{2}}\langle\Psi_{\mathcal{R}'}, \textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x}\right)\Psi_{\mathcal{R}}\ dk\rangle + \alpha^2\langle\Psi_{\mathcal{R}'}, V(\alpha x)\Psi_{\mathcal{R}}\rangle. \\
\\
&= \langle\nabla_x\Psi_{\mathcal{R}'}, \nabla_x\Psi_{\mathcal{R}}\rangle + \textstyle\int_{\mathbb{R}^3}\langle\Psi_{\mathcal{R}'}, a_k^\dagger a_k\Psi_{\mathcal{R}}\rangle dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\langle\Psi_{\mathcal{R}'}, \left(a_k e^{ik\cdot x} + a_k^\dagger e^{-ik\cdot x}\right)\Psi_{\mathcal{R}}\rangle dk + \alpha^2\langle\Psi_{\mathcal{R}'}, V(\alpha x)\Psi_{\mathcal{R}}\rangle. \\
\\
&= \langle\nabla_x\Psi_{\mathcal{R}'}, \nabla_x\Psi_{\mathcal{R}}\rangle + \textstyle\int_{\mathbb{R}^3}\langle a_k\Psi_{\mathcal{R}'}, a_k\Psi_{\mathcal{R}}\rangle dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\langle\Psi_{\mathcal{R}'}, a_k e^{ik\cdot x}\Psi_{\mathcal{R}}\rangle + \langle a_k e^{ik\cdot x}\Psi_{\mathcal{R}'}, \Psi_{\mathcal{R}}\rangle\right)dk + \alpha^2\langle\Psi_{\mathcal{R}'}, V(\alpha x)\Psi_{\mathcal{R}}\rangle \\
\\
&= \langle\Phi(\mathcal{R}'\cdot), \Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\nabla_x\varphi(\mathcal{R}'x), \nabla_x\varphi(\mathcal{R}x)\rangle_e \\
&+ \textstyle\int_{\mathbb{R}^3}\langle\varphi(\mathcal{R}'x), \varphi(\mathcal{R}x)\rangle_e\langle a_k\Phi(\mathcal{R}'\cdot), a_k\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\, dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\langle\varphi(\mathcal{R}'x)\Phi(\mathcal{R}'\cdot),\ a_k\Phi(\mathcal{R}\cdot)e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle\right)dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\langle a_k\Phi(\mathcal{R}'\cdot)e^{ik\cdot x}\varphi(\mathcal{R}'x),\ \varphi(\mathcal{R}x)\Phi(\mathcal{R}\cdot)\rangle\right)dk \\
&+\langle\Phi(\mathcal{R}'\cdot), \Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\varphi(\mathcal{R}'x),\ \alpha^2 V(\alpha x)\varphi(\mathcal{R}x)\rangle_e \\
\\
&= \langle\Phi(\mathcal{R}'\cdot), \Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\nabla_x\varphi(\mathcal{R}'x), \nabla_x\varphi(\mathcal{R}x)\rangle_e \\
&+ \textstyle\int_{\mathbb{R}^3}\langle\varphi(\mathcal{R}'x), \varphi(\mathcal{R}x)\rangle_e\langle\frac{z_\varphi(\mathcal{R}'k)}{|k|}\Phi(\mathcal{R}'\cdot), \frac{z_\varphi(\mathcal{R}k)}{|k|}\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\ dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\langle\varphi(\mathcal{R}'x)\Phi(\mathcal{R}'\cdot), \frac{z_\varphi(\mathcal{R}k)}{|k|}\Phi(\mathcal{R}\cdot)e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle\right)dk \\
&+\alpha^{\frac{1}{2}}\textstyle\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\langle\frac{z_\varphi(\mathcal{R}'k)}{|k|}\Phi(\mathcal{R}\cdot)e^{ik\cdot x}\varphi(\mathcal{R}'x), \varphi(\mathcal{R}x)\Phi(\mathcal{R}\cdot)\right)dk
\end{aligned}$$

$+\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\varphi(\mathcal{R}'x),\alpha^2V(\alpha x)\varphi(\mathcal{R}x)\rangle_e.$

$= \langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\left(\int_{\mathbb{R}^3}\nabla_x\varphi(\mathcal{R}'x)\overline{\nabla_x\varphi(\mathcal{R}x)}dx\right)$

$+\int_{\mathbb{R}^3}\langle\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\frac{\overline{z_\varphi(\mathcal{R}k)}z_\varphi(\mathcal{R}k)}{|k|^2}\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\frac{\overline{z_\varphi(\mathcal{R}k)}}{|k|}\langle\varphi(\mathcal{R}'x)\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle\right)dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\frac{\overline{z_\varphi(\mathcal{R}'k)}}{|k|}\langle\Phi(\mathcal{R}'\cdot)e^{ik\cdot x}\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\Phi(\mathcal{R}\cdot)\right)dk$

$+\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\varphi(\mathcal{R}'x),\ \alpha^2V(\alpha x)\varphi(\mathcal{R}x)\rangle_e$

$= \langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\left(\int_{\mathbb{R}^3}\nabla_x\varphi(\mathcal{R}'x)\overline{\nabla_x\varphi(\mathcal{R}x)}dx\right)$

$+\int_{\mathbb{R}^3}\langle\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\frac{\overline{z_\varphi(\mathcal{R}'k)}z_\varphi(\mathcal{R}k)}{|k|^2}dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\frac{\overline{z_\varphi(\mathcal{R}k)}}{|k|}\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle\varphi(\mathcal{R}'x),e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle_e\right)dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\left(\frac{z_\varphi(\mathcal{R}'k)}{|k|}\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\langle e^{ik\cdot x}\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\right)dk$

$+\alpha^2\langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\int_{\mathbb{R}^3}\varphi(\mathcal{R}'x)V(\alpha x)\overline{\varphi(\mathcal{R}x)}dx$

$= \langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\Big[\int_{\mathbb{R}^3}\nabla_x\varphi(\mathcal{R}'x)\overline{\nabla_x\varphi(\mathcal{R}x)}dx+$

$+\langle\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\int_{\mathbb{R}^3}\frac{\overline{z_\varphi(\mathcal{R}'k)}z_\varphi(\mathcal{R}k)}{|k|^2}dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\frac{\overline{z_\varphi(\mathcal{R}k)}}{|k|}\langle\varphi(\mathcal{R}'x),e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle_e\,dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\frac{z_\varphi(\mathcal{R}'k)}{|k|}\langle e^{ik\cdot x}\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\,dk$

$+\alpha^2\int_{\mathbb{R}^3}\varphi(\mathcal{R}'x)V(\alpha x)\varphi(\mathcal{R}x)dx\Big]$

$= \langle\Phi(\mathcal{R}'\cdot),\Phi(\mathcal{R}\cdot)\rangle_{\mathcal{F}}\Big[\int_{\mathbb{R}^3}\nabla_x\varphi(\mathcal{R}'x)\overline{\nabla_x\varphi(\mathcal{R}x)}dx+$

$+\alpha\langle\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\int\int_{\mathbb{R}^3\times\mathbb{R}^3}\frac{\varphi^2(\mathcal{R}x)\overline{\varphi^2}(\mathcal{R}'y)}{|x-y|}\,dxdy$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\frac{\overline{z_\varphi(\mathcal{R}k)}}{|k|}\langle\varphi(\mathcal{R}'x),e^{ik\cdot x}\varphi(\mathcal{R}x)\rangle_e\,dk$

$+\alpha^{\frac{1}{2}}\int_{\mathbb{R}^3}\frac{1}{|k|}\frac{z_\varphi(\mathcal{R}'k)}{|k|}\langle e^{ik\cdot x}\varphi(\mathcal{R}'x),\varphi(\mathcal{R}x)\rangle_e\,dk$

$+\alpha^2\int_{\mathbb{R}^3}\varphi(\mathcal{R}'x)V(\alpha x)\varphi(\mathcal{R}x)dx\Big]$ and

$\int\int_{SO(3)\times SO(3)}d\gamma(\mathcal{R})\,d\gamma(\mathcal{R}')\lim_{\alpha\to\infty}\left(\frac{\langle\Phi(\mathcal{R}\cdot),\Phi(\mathcal{R}'\cdot)\rangle_{\mathcal{F}}}{\langle\overline{\Psi}_\rho,\overline{\Psi}_\rho\rangle}\right)\times$

$\times\Big[\int_{\mathbb{R}^3}\nabla\phi(\mathcal{R}'x)\overline{\nabla\phi(\mathcal{R}x)}dx+$

$$
\begin{aligned}
&+\langle\phi(\mathcal{R}x),\,\phi(\mathcal{R}'x)\rangle_e \int\int_{\mathbb{R}^3\times\mathbb{R}^3} \tfrac{\phi^2(\mathcal{R}x)\overline{\phi^2(\mathcal{R}y)}}{|x-y|}dx\,dy+\\
&-\int_{\mathbb{R}^3} \tfrac{\widehat{|\phi_{\mathcal{R}}|^2}(k)}{|k|^2}\langle\phi(\mathcal{R}'x),\,e^{ik\cdot x}\phi(\mathcal{R}x)\rangle_e dk+\\
&-\int_{\mathbb{R}^3} \tfrac{\widehat{|\phi_{\mathcal{R}'}|^2}(k)}{|k|^2}\langle e^{ik\cdot x}\phi(\mathcal{R}'x),\,\phi(\mathcal{R}x)\rangle_e dk+\\
&+\int_{\mathbb{R}^3}\phi(\mathcal{R}'x)V(x)\overline{\phi}(\mathcal{R}x)\,dx\Big]\\
=\;& e_P(V)
\end{aligned}
$$

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